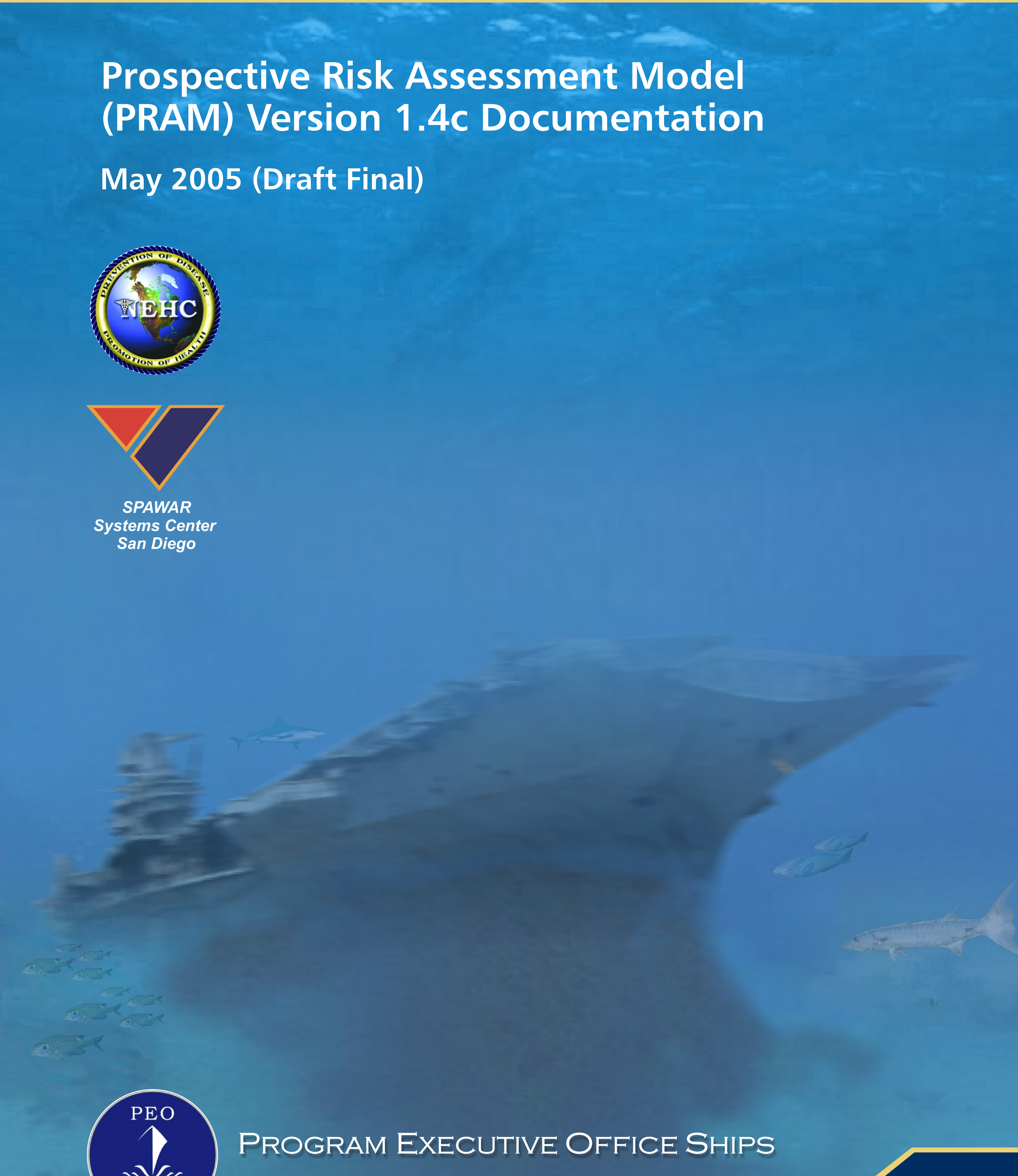
Artificial Reefing



Prospective Risk Assessment Model (PRAM) Version 1.4c Documentation

May 2005 (Draft Final)

NEHC
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Prospective Risk Assessment Model (PRAM) Version 1.4c Documentation

May 2005 (Draft Final)

SPAWAR
Systems Center
San Diego

URS

May 16, 2005

Mr. Chris Gluck (CENWS-EC-TB-ET)
U.S. Army Corps of Engineers – Seattle District
4735 East Marginal Way South
Seattle, WA 98101

Subject: Polychlorinated Biphenyl (PCB) Risk Assessment at Sunken Navy Vessel Artificial Reef
Contract No. DACA67-02-D-2003, Delivery Order No. 0027
Modification 02

Re: Transmittal of Deliverables

Dear Mr. Gluck:

We are pleased to provide the Draft Final Prospective Risk Assessment Model (PRAM) (version 1.4) and its documentation. Per Modification 02 to Delivery Order No. 0027, a total of 9 hard copies of the PRAM and Time Dynamic Model (TDM) documentation are enclosed. An additional 15 electronic copies (on CD) are also provided, which contain all three documents. This deliverable includes the following:

- PRAM Version 1.4
- PRAM Documentation
- TDM Documentation

Should you have any questions concerning this matter, please contact me at 206.438.2322 or Peter Tong at 312.697.7228. We thank you for the opportunity to service the Navy through your contract.

Sincerely,

Kara Steward
Administrative Project Manager

Peter Tong, CEA, CHMM, REM
Technical Project Manager

cc: Elizabeth Freese (NAVSEA PM333)
Bill Wild (SPAWARSYSCEN-SD)
Yvonne Walker (NEHC)

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EPA Headquarters
Laura Casey, Office of Pollution Prevention and Toxics, OPPTS
Dr. Linda Phillips, Office of Science Coordination and Policy, OPPTS
Dr. Laura Johnson, Office of Wetlands, Oceans, and Watersheds, OW

EPA Region 4
Craig Brown, PCB Program, Air, Pesticides, and Toxics Management Division
Dr. Kenneth Mitchell, Regional Human Health and Ecological Risk Assessor, Air, Pesticides, and Toxics Management Division

EPA Environmental Effects Research Laboratory
Dr. Wayne Munns, Atlantic Ecology Division – Narragansett EERL

EPA National Exposure Research Laboratory
Dr. Craig Barber, Ecosystems Division – Athens NERL

Florida Fish and Wildlife Conservation Commission
Jon Dodrill, Artificial Reef Program, Division of Marine Fisheries, FFWCC

Florida Escambia County
Robert Turpin, Marine Resources Division

Florida Department of Health and Rehabilitative Services
Dr. Joseph Sekerke, Office of Toxicology and Hazard Assessment

Florida Executive Office of the Governor
Debbie Tucker, Office of Environmental Affairs

This document is dedicated to the memory of our good friend and colleague, Mark Seth Goodrich (1957 – 2005), primary modeler and author of the PRAM.

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ACRONYMS AND ABBREVIATIONS

ATSDR	Agency for Toxic Substances and Disease Registry
BAF	biological accumulation factor
BCF	bioconcentration factor
CalTOX	California EPA Multimedia Total Exposure Model for Hazardous Waste Sites
CFR	Code of Federal Regulations
CNO	Chief of Naval Operations
COC	constituent of concern
CTE	central tendency exposure
deca-CBs	PCB congeners with 10 of 10 possible chlorine substitutions
DO	dissolved oxygen
DOC	dissolved organic carbon
ECETOC	European Centre for Ecotoxicology and Toxicology of Chemicals
f	fugacity
FI	fraction of fish ingested
FWCC	Florida Fish and Wildlife Conservation Commission
FWR	Final Weight Report
g	gram
GUI	Graphical User Interface
hexa-CBs	PCB congeners with 6 of 10 possible chlorine substitutions
IR	ingestion rate
IRIS	Integrated Risk Information System
kg	kilogram
K_{oc}	water to particulate organic carbon partitioning coefficient
K_{doc}	water to dissolved organic carbon partitioning coefficient
K_{ow}	octanol to water partitioning coefficient
LAARS	large area artificial reef site
LLNL	Lawrence Livermore National Laboratory
m	meter
MAMES	Mississippi-Alabama Marine Ecosystem Study
mg	milligram
MMS	Minerals Management Service
mol	mole
mono-CBs	PCB congeners with 1 of 10 possible chlorine substitutions
NAVSEA	Naval Sea Systems Command
NDBC	National Data Buoy Center

ACRONYMS AND ABBREVIATIONS (Continued)

NEHC	Navy Environmental Health Center
ng	nanogram
NMFS	National Marine Fisheries Service
NOAA	National Oceanic and Atmospheric Administration
nona-CBs	PCB congeners with 9 of 10 possible chlorine substitutions
Pa	Pascals
PCB	Polychlorinated Biphenyl
PRAM	Prospective Risk Assessment Model
QSAR	Quantitative structure activity relationship
RAGS	Risk Assessment Guidance for Superfund
REEFEX	Reef Exercise (Sunken Vessels Used to Construct Artificial Reefs on the Continental Shelf of the US)
RfD	reference dose
RISC	Risk-Integrated Software for Clean-ups
RME	reasonable maximum exposure
SCEM	Site Conceptual Exposure Model
SF	slope factor
SHHRA	Supplemental Human Health Risk Assessment
SINKEX	Sinking Exercise (Sunken Vessel Exercise, same as the Navy's Deep Water Sinking Program)
SSC-SD	Space and Naval Warfare Systems Center (SPAWARSYSCEN) San Diego, an organization of the Space and Naval Warfare Systems Command (SPAWAR)
SPAWAR	Space and Naval Warfare
TDM	Time-dynamic model
TL	Trophic Level
TWG	Technical Working Group
UCD	University of California – Davis
UCL	Upper confidence limit
USEPA	U.S. Environmental Protection Agency
USGS	United States Geological Survey
ZOI	Zone of Influence

A Prospective Risk Assessment Model (PRAM) has been developed under the technical direction of the Navy Environmental Health Center (NEHC), Portsmouth, Virginia, to facilitate the evaluation of decommissioned ex-Navy vessels as potential artificial reef building material.[1] NEHC is the Navy Surgeon General's organization for population health and environmental health risk assessments, and a technical advisor to the Chief of Naval Operations (CNO). The funding proponent for PRAM is CNO's Naval Sea Systems Command (NAVSEA) Inactive Ships Program Office (PMS 333). Project management is assisted by the Space and Naval Warfare (SPAWAR) Systems Center, San Diego (SSC-SD), which is the CNO's center of expertise on scientific research and ecological risk assessments.

1.1 MODEL BACKGROUND AND DEVELOPMENT

The development of the PRAM followed the process guidance of Mackay et al., 1995, as shown in Figure 1 and summarized below.

The original "problem" was defined as, "What are the potential human health risks associated with the presence of residual polychlorinated biphenyls (PCBs) onboard a sunken-vessel artificial reef and the potential for transfer of these PCBs into edible aquatic species associated with the reef and their subsequent consumption by recreational anglers?"

The PRAM has been designed to estimate, under various physical and environmental conditions, the potential exposure concentrations in edible sports fish associated with the sunken vessel as an artificial reef. The PRAM predictions reflect the incremental risk associated with the vessel artificial reef; they do not include or determine the background[2] risks of PCBs in the general marine environment. The approach used in PRAM is to assure a reasonable estimate of the transfer of PCBs for use to assess risks under reasonable maximum exposure and central tendency conditions.

The initial concept of a prospective risk assessment in the context of artificial reef building with ex-Navy vessels was presented at an interagency Technical Working Group (TWG)[3] meeting in 1999. The purposes were to "bound" the problem, as perceived by the Navy, and

[1] This document is prepared by URS Corporation.
[2] Background referring to the in-situ concentration of PCBs within the system prior to the deployment of a vessel for artificial reef building.
[3] The SINKEX/REEFEX interagency Technical Working Group (TWG) was comprised of U.S. Environmental Protection Agency (USEPA) representatives from the Office of Pollution Prevention and Toxics (USEPA OPPT), Navy representatives, and contractors to the Navy.

present the conceptual/process design. After the initial introduction the concept was briefed to the Navy as follows:

> *"An assessment of risk that is based on known/estimated contaminant source values, modeled fate and transport values, and assumptions about exposure pathways and extent of exposure"* (A. Lunsford, NEHC – RDML L.C. Baucom Briefing, February 23, 2000).

An initial demonstration program, with all of the relevant equations considered at that time, was developed and presented to the REEFEX/SINKEX TWG in 2000. The modeling algorithms and mathematical assumptions used in that PRAM version were extensively reviewed by NEHC in late 2000 and early 2001, after which a formal sensitivity analysis was performed on the list of variables within the PRAM. Later in 2001, draft leachate rates of PCB-containing bulk product materials developed by the SSC-SD Marine Environmental Support Office were incorporated into the PRAM and an external peer review was performed by the Research Triangle Institute (RTI), Research Triangle Park, North Carolina. This review resulted in, among other things, the incorporation of a compartment, interior to the sunken vessel, into which PCBs are initially released. Comments presented by external reviewers (non-Navy TWG representatives) were addressed in that same year. A preliminary risk assessment was performed using data obtained from the ex-AGERHOLM (a Gearing class destroyer [DD-826], deployed in deep water off the coast of California) and presented for peer review at the Second International Conference of Contaminated Sediments, Venice, Italy (Goodrich et al., 2003).

In 2004, updated PCB homolog-specific leachate rates were provided by SSC-SD and incorporated into PRAM, and a number of parameters (for example, vessel dimensions, PCB source material amounts, and water column height) were changed to make the model specifically applicable to the proposed ex-ORISKANY[4] Memorial Reef. This revised PRAM (Version 1.3) was developed to estimate the potential impact associated with the deployment of the ex-ORISKANY as an artificial reef. The PRAM (Version 1.3) was provided to the USEPA[5] and State of Florida representatives for review in July 2004.

4 Ex-ORISKANY (CVA-34) is the last Essex class aircraft carrier that served the Navy fleet for more than 25 years, maintaining a powerful presence during the Korean War and the Vietnam conflict. It was decommissioned in 1976.

5 The PRAM (Version 1.3) was provided to EPA Region 4, EPA Headquarters, EPA OPPT, and EPA National Exposure Research Laboratory (NERL) representatives for review.

Technical enhancements added to PRAM Version 1.3 to develop Version 1.4c are addressed in Section 1.3. The following section provides a generalized description of PRAM.

1.2 GENERALIZED DESCRIPTION OF PRAM

This generalized description of PRAM is provided for readers who are interested in having a general overview of the model. In Sections 2, 3, and 4 of this document, more scientific and detailed descriptions of the model's construct, algorithms, and assumptions are provided.

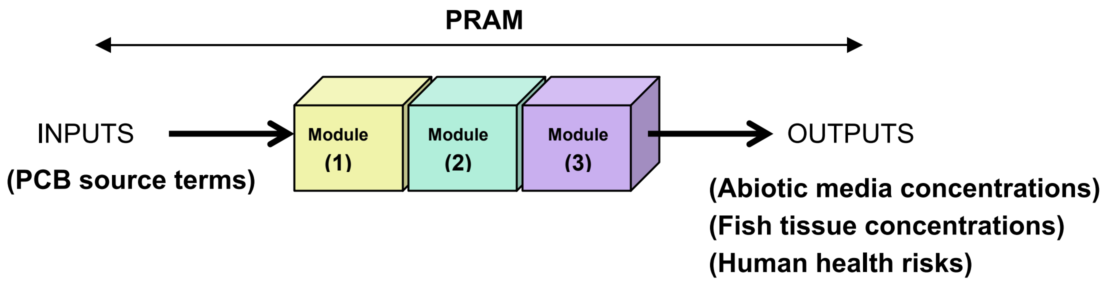
1.2.1 Introduction

One of the most important things to note about the Navy's PRAM is that it is much more than just a "risk assessment" model. The risk assessment portion actually constitutes only one module of the model.

Within PRAM there are at least three constituent modules: a multimedia, environmental chemical fate model, a biological uptake and bioaccumulation model, and a risk characterization model. These three models are directly linked together within PRAM, such that the model begins with a known quantity of a chemical, or known quantities of several chemicals (chemical source terms), simulates how these chemicals will be distributed within a marine environment, simulates how the chemicals will be taken up and bioaccumulated in living organisms, and finally, calculates the human health risks (carcinogenic risks and non-cancer hazards) that would be associated with consuming fish that have accumulated those chemicals. Thus the PRAM can be viewed as a series of interconnected models (Figure 2).

1.2.2 Generalized Model Construct

For purposes of this general discussion, the PRAM is described as consisting of three underlying models, or modules, and as having a specific starting point (an initial "input" area) and a specific stopping point (an "output," or results area), as illustrated below:



In the above illustration:

- "Inputs" to the PRAM are the chemical source terms specific to a particular sunken vessel. For the ex-ORISKANY risk assessment, the primary chemical of concern is PCBs. The amount of each PCB homolog (mono- through deca-chlorobiphenyl) remaining in materials onboard the ex-ORISKANY when it is deployed as an artificial reef are the source terms (inputs) to PRAM for this assessment.

- "Module 1" is the multimedia environmental model of chemical fate. This section of PRAM incorporates the equations and physical parameters that govern the processes by which PCB homologs are released and disbursed in the marine environment surrounding the sunken vessel, and distributed into the various abiotic media compartments (water, suspended solids, dissolved organic carbon, sediment, and air) within a defined volume around the sunken vessel.

- "Module 2" is the biotic-food web and bioaccumulation model, which we call the PRAM biotic-food web module. This section of PRAM incorporates the equations and parameters that govern the processes by which the PCB homologs that have been distributed into the various media compartments make their way into living organisms, make their way up through the food chain, and are accumulated in the tissues of marine biota such as algae, phytoplankton and zooplankton, benthic organisms, and reef fish species.

- "Module 3" is the risk characterization model. This section of PRAM incorporates the equations and parameters that are used to assess human health risks, based on a specific exposure scenario, i.e., human consumption of reef-associated fish that have accumulated PCBs within their tissues, and the inherent toxicity of PCBs.

- “Outputs” of the PRAM can be viewed as occurring at many points. The “output spreadsheet” of the model indicates the values that have been calculated at various points in PRAM. For example, the PRAM “output spreadsheet” records the PCB concentrations that have been calculated for air, water, dissolved organic carbon, suspended solids, and bedded sediments within the defined exposure zone; the bioaccumulation factors that have been calculated for various fish species associated with the reef environment; the tissue concentrations that have been calculated for biota such as algae, phytoplankton, zooplankton, planktivores and piscivores, including edible reef fish species associated with the reef environment; and (the final outputs for PRAM), the human health risk values (cancer risk and non-cancer hazard estimates), for both adults and children, that are associated with chronic ingestion of each representative reef fish.

The above description is, of course, a simplified description of the PRAM, provided for purposes of this general discussion. In Section 2 of this document (“Model Assumptions”), a more scientific and detailed description of the model is given.

1.2.3 Rationale for PRAM Development

Readers may wonder why the PRAM was developed. They may ask: Was it necessary to develop a new environmental model to assess the potential risks associated with sunken vessels being used as artificial reefs? Are there not many existing environmental fate and transport models available? Are there not many risk assessment models available? Could one of these existing models have been used?” The following discussion is provided to answer these questions.

The PRAM was developed in order to be able to assess the potential risks, to human health and the environment, that could be associated with deploying decommissioned ships as artificial reefs. The obvious problem presented by this scenario is that there is a need to assess the potential risk before the vessel is sunk. Many environment risk assessments (for example, the “Superfund” risk assessments) are conducted after the fact, such that soil, air, water, or sediment samples, and even biological samples, can be collected to determine whether these media are impacted by pollutants that were released some time in the past. Many risk assessment software programs thus have “input” areas into which one inputs the concentrations of chemicals that were found in abiotic or biotic media. A prospective risk assessment, on the other hand, must model how an anticipated chemical release at a given locality and a specific point in time might distribute itself within the receiving environment and make its way into an ecosystem or food chain. The concentrations that will result in abiotic and biotic media must be simulated, by modeling the distribution of the chemical as accurately as possible.

1.2.4 Constructing the PRAM

Another problem presented by the artificial reef modeling scenario is the lack of pre-existing marine models for this type of assessment. Most of the existing environmental fate and transport models were developed to track chemicals that were initially released on land, or into the air, or into a fresh water body such as a lake or river. In the context of the Artificial Reefing Program, the focus is on tracking the fate of chemicals that might be released from a sunken vessel, into a marine environment. The marine ecosystem presents a “receiving” environment that is significantly different from land-based or fresh water body-based scenarios.

One important consideration in a marine model is that there are few, if any, limiting physical boundaries anticipated in an ocean environment (e.g., no nearby walls, or stream banks, or other barriers). The limiting “boundaries,” for tracking the fate of a chemical released in the ocean, are physical processes such as ocean currents, and tides, and the sheer volume of water into which chemicals are released; chemical/physical properties such as the solubilities of different chemicals; diffusion limitations; and the capacities of the various media within the marine environment to adsorb or absorb the chemicals. Within the ocean, currents and tides act to “sweep away” chemicals from the point of release, while abiotic media compartments, such as sediment, act to adsorb chemicals that have dissolved in the water. At some point in time, given the vastness of the ocean, the chemicals which have been dissolved in the water, and which have not been absorbed into the sediment or other media compartments, will be distributed over such a large volume of water that the concentrations will reach “background” or undetectable levels. Thus, for a chemical fate and transport model pertaining to an ocean environment, there is a need to define a relevant “exposure zone,” or “zone of influence” around the point of release, within which marine organisms may be assumed to be exposed to higher-than-background levels of the chemical.

Another complexity associated with modeling chemical fate and transport in a marine environment is the lack of specific information about the “mass” of living organisms that may live within, or routinely enter, the defined volume of the "exposure zone." Many environmental fate-and-transport models use "mass-balanced" equations. In order to use these algorithms, the masses of all compartments within the model must be known. At a minimum, one should at least have good estimates of the masses, such that there will not be a high level of uncertainty associated with the model's results. Currently, there are no reliable estimates of the "mass" of biota around an artificial reef. This is due to a number of factors. Artificial reefs vary significantly from one another in both size and shape. They are deployed at differing water depths, and are located nearer or farther away from coast lines and estuary outfalls. Colonization rates on artificial reefs differ significantly from one region of the ocean to another, depending on ambient water temperatures and other factors. Fish varieties and abundances differ from one region to another and with ocean depths. These and other factors contribute to a lack of specific knowledge about the mass of biota that can be expected to occur at any given artificial reef site.

In researching available environmental chemical fate models, it was discovered that fugacity-based environmental models circumvented the need to have precise values for biota masses. In particular, the Mackay fugacity-based models (Mackay, 2001) use an approach that is scientifically sound, and that has been published, peer reviewed, and used in several environmental assessments. For example, this approach was used by the U.S. EPA in developing the Great Lakes Water Quality Criteria. Since the fugacity approach does not require estimates/values of biotic mass, this seemed an ideal approach for use in modeling chemical fate in a marine environment. Within PRAM, we have used the Mackay fugacity approach to model chemical fate in a marine environment. Specifically, a "Level III Fugacity Model" was used. This is described in Section 2 of this document.

After modeling the chemical fate of PCB homologs in a marine environment, the next module in PRAM is the biological uptake and bioaccumulation model. In order to determine the concentrations of PCBs that can be expected in biological organisms that are associated with the artificial reef, an appropriate biotic-food web and bioaccumulation model was needed. Here again, while there are established and accepted methods to estimate biouptake and bioaccumulation in fish and other biota, no appropriate off-the-shelf model could be found that could be used in the artificial reef context. Specifically, no models were found that were constructed to estimate biouptake and bioaccumulation in a variety of marine organisms coexisting in a delimited ocean environment.

To model biouptake in a variety of marine fish, for example, one must have information about the energy budgets of representative marine fish species (i.e., what fraction of their energy is used for respiration?, what fraction is used for growth and reproduction?, what fraction is used for excretion?) and information about their biological makeup (average adult body weight, fraction of lipid content, fraction of water content, average caloric intake, fraction of metabolizable energy relative to gross energy). One needs to know, or have the appropriate data to calculate the respiration rates of different representative species. One needs to have information about their diets (e.g., fraction of suspended solids in diet, fraction of phytoplankton in diet, fraction of zooplankton in diet, fraction of sessile filter feeders, and fractions of infaunal and epifaunal benthos in diet, fractions of benthic foragers and reef/vessel foragers in diet). While well known and accepted equations were used in the biotic-food web and bioaccumulation model in PRAM, the model itself had to be constructed, to include representative species at four trophic levels within each of three different communities associated with artificial reefs (pelagic community, reef-associated community, and benthic community). Published scientific literature had to be searched to find data on energy budgets associated with different representative species, and their diet fractions, and respiration rates, and their physical makeup (lipid and water fractions, etc.). In many cases, consensus on specific parameters, such as diet fraction or respiration rates, needed to reached with model reviewers, marine biologists, and other personnel that participated in a Technical Working Group (a technical advisory body). This section of PRAM was essentially constructed de novo, using algorithms and data from a number of sources.

The final section of PRAM, the human health risk assessment section, is the most straightforward of the three constituent models within PRAM, with respect to its adherence to, and direct incorporation of, pre-established algorithms and input parameters for risk assessment. The equations used in the human health risk assessment section are directly reproduced from the U.S. EPA publication "Risk Assessment Guidance for Superfund" (RAGS). The RAGS document provides example equations for assessing human health risks based on a variety of exposure scenarios, including a fish consumption exposure scenario. Other well-known U.S. EPA guidance documents such as the *Exposure Factors Handbook* (1997) were used as reference sources for input parameters such as the average and upperbound fish ingestion rates for the Gulf States. The only parameter within the fish consumption scenario risk equations that needed to be determined specifically for the ex-ORISKANY risk assessment was a locality-specific "fraction ingested" (FI) value. The FI value pertains to the fraction of fish that would be caught at the artificial reef and consumed by a sports angler and/or his family as compared to the total amount of fish (from all sources, including fish eaten at restaurants or purchased from a grocer) that would be expected to be consumed by the sports angler and his family. An Escambia County-specific FI value was derived empirically, by conducting a Fish Consumption Survey of sports fishermen in Escambia County.

1.2.5 PRAM Format and User Interface

PRAM was developed with Microsoft Excel™ software, and Visual Basic++™. All of the equations and input parameters used in the model are resident in the Excel database that is supported by a Graphical User Interface (GUI). The database and GUI are provided as a bundled electronic file titled "PRAM, Version 1.4c." Electronic copies of the model have been provided to cognizant personnel at the U.S. EPA, the State of Florida, and the U.S. Navy.

The GUI of PRAM provides users with many options. An opening screen is displayed, from which the user can choose to either "run" the program (using default values that are already incorporated in the model) to obtain estimates of PCB concentrations in abiotic and biotic media, and estimates human health risks, or to view the individual "modules" that comprise the PRAM, and the various equations, parameters, and values that are used in each of the modules. If the user wishes, input parameter values can be changed; for example the "lipid fraction" of a given representative biological organism can be changed, or a different mass of PCB source material could be used. Also, users can reset input parameters to the default values.

1.2.6 Empirical Data Used in PRAM

In addition to data that was gleaned from published scientific literature, PRAM uses empirical data from three significant sources:

- The December 7, 2004 CACI report, "Final Report, Revision 4, Polychlorinated biphenyls (PCB) Source Term Estimates for ex-ORISKANY (CVA-34)"
- The October, 2004 SPAWARS SSC-SD report, "Draft Final Report: Investigation of Polychlorinated Biphenyl (PCB) Release-Rates from Selected

Shipboard Solid Materials Under Laboratory-Simulated Shallow Ocean (Artificial Reef) Environments"

- The June, 2004 Escambia County, FL report, "Escambia County Fish Consumption Survey"

1.3 VERSIONS OF THE PRAM MODEL

The history in Section 1.1 takes the PRAM through Version 1.3 and brings us to the point in the development process (Figure 1) where one could ask, "Are revisions required to satisfy the model objectives?" USEPA and other reviewers raised several issues and concerns that led to recommendations to further revise the PRAM. In response, significant modifications were made to PRAM (Version 1.3), resulting in PRAM Version 1.4c. This document presents the technical details of this latest version.

Changes made from PRAM Version 1.3 (July 2004) to Version 1.3c (September 2004) included:

1. Incorporating a child receptor into the risk characterization module.
2. Updating default values, to reflect ex-ORISKANY-specific exposure scenario.
3. Fixing typographical errors in PRAM Version 1.3 modules for solving to non-risk PCB load onboard and risk estimates for range of PCB loads onboard.
4. Reprogramming PRAM to provide additional outputs from the model, including: bioaccumulation factors calculated for each trophic level for each homolog series; feeding rates calculated for each trophic level; and growth rates calculated for each trophic level.
5. Incorporating revised leachate rate data (from SSC-SD) into the model.
6. Adding a factor to account for metabolizable energy, versus gross energy, of dietary items.

Changes made from PRAM Version 1.3c (September 2004) to Version 1.4c (May 2005) included:

1. Revising fish respiration parameters to reflect marine species.

2. Incorporating gill efficiency "correction" for PCB uptake rates in fish.
3. Refining algorithms to achieve Level III fugacity, versus using a Level II fugacity approach.
4. Incorporating a pycnocline boundary condition with the water column, and division of the external water column into two layers (i.e., into upper, epilimnion layer and lower, hypolimnion layer).
5. Revising the biotic-food web module for the lower epilimnion layer and designing a new biotic-food web module for the upper epilimnion layer (Appendix G), per diet-water exposure matrix table developed with TWG.
6. Constructing an interface or macro to receive TDM abiotic media concentration output to estimate biota concentrations in water column (see Time Dynamic Model [TDM] Documentation for details).
7. Incorporating multiple zones of influence per negotiated agreement established in the TWG based on feeding behavior, range and habitat of relevant fish species of concern.
8. Modifying the GUI to provide input values to parameters and to generate output from the model, based on the above structural modifications.
9. Conducting quality assurance check, testing, and sensitivity analysis.

1.4 PURPOSE

This document, short-titled, "Prospective Risk Assessment Model (PRAM) Version 1.4c Documentation" provides model objectives and background information, and details the scientific basis, model structure, assumptions, input parameters, output, findings of limited testing and sensitivity analysis, and uncertainties/limitations of PRAM Version 1.4c. The purpose is to provide background and technical information to USEPA, State of Florida, and external reviewers on PRAM Version 1.4c that was revised from earlier versions (1.3 and 1.3c) in response to comments and resolution of issues by the TWG. In addition, this document serves as a basis for performance of a revised Supplemental Human Health Risk Assessment (SHHRA; revised from the July 2004 SHHRA), using PRAM (Version 1.4c) in support of seeking a risk-based approval from USEPA per 40 CFR 761.62 (c).

This document is not intended as a user manual for modelers or risk assessors who want to use PRAM to estimate human health risks for future vessels, ascertain mass/volume reduction of PCB–containing bulk products of other vessels to achieve an acceptable risk level, or the generation of PCB concentrations in biota based on site-specific environmental conditions and PCB loading information of vessels other than the ex-ORISKANY. This document is a compendium document for "Time Dynamic Model (TDM) Documentation" that addresses using the Time Dynamic Model developed by SSC-SD, in combination with the biotic-food web module of PRAM (Version 1.4c) to evaluate human health and ecological risks in the early stage (transient or pulse-release period) of a sunken artificial reef vessel before steady-state PCB release and transport conditions are reached.

1.4.1 Model Objectives

As a multimedia environmental fate and transport and risk assessment model, PRAM (Version 1.4c) has two objectives:

- Predict human health risks from the fish ingestion pathway of anglers at or near the ex-ORISKANY artificial reef under steady-state and chronic-exposure conditions.

  The fugacity Level III fate and transport module in PRAM will estimate the PCB concentrations in the various abiotic media in the marine environment surrounding the reef under a steady-state condition, at about two years after the sinking of the vessel, up to an unlimited (undefined) amount of time.

- Estimate PCB concentrations in a variety of representative biological species that reside on or near the artificial reef during the transient or pulse-release time period.

  As described in the Time Dynamic Model (TDM) Documentation, the PRAM's biotic-food web module has been modified so that it can process abiotic concentrations or output predicted by TDM to produce PCB concentrations in biota during the transient or pulse-release time period, defined as 0 to 2 years after deployment of the ex-ORISKANY as an artificial reef. The calculated biota concentrations can then be used to evaluate human health and ecological risks.

1.4.2 Need for Predictive Modeling

Human health and ecological risk assessments associated with using the vessel as an artificial reef must be conducted before the ex-ORISKANY is deployed. This is because the USEPA must first issue a risk-based PCB Disposal Approval under 40 CFR 761.62 (c). This presents a problem because there are no “potentially contaminated samples” to collect or investigate. Until the vessel is sunk, there is no known source of PCB-containing bulk product materials nor reef-associated biological communities at the proposed site. Eventually, a variety of biological organisms, such as fish, algae, and bivalves will associate with or attach themselves to the reef. In consultation with USEPA and Florida through the TWG, the Navy does not know of readily available model(s) that can be used to satisfy requirements for the demonstration of unacceptable risks under the USEPA risk-based approval process.

Thus, there is a compelling need to use a multimedia environmental simulation model to predict abiotic and biotic media concentrations for the ex-ORISKANY artificial reef.

Predictive modeling using PRAM has been developed to assess how an anticipated PCB release from a sunken vessel might distribute itself within the receiving environment and make its way into the ecosystem and food chain, both during the period when the reef is being colonized, and after a fully matured, viable reef has been established. However, PRAM’s fate and transport module is based on a steady-state condition in terms of the thermodynamic principles that govern fate and transport of a chemical in the environment. To address the initial or transient environmental conditions (i.e., pulse-release concern) expressed by reviewers of PRAM (Version 1.3), the TDM developed by SSC-SD is used to generate abiotic media within the marine environment at specific periods of time after vessel deployment, and at specific distance intervals from the sunken vessel. By incorporating the TDM output in terms of average abiotic concentrations in a quasi-time dynamic scale (via multiple steps in time and space), PRAM’s biotic-food web module can be used to evaluate the potential human health and ecological risks in the transient period (see TDM Documentation).

TDM and PRAM are based on scientifically sound and widely accepted physical and biological algorithms and models. As such, they are predictive mathematical modeling tools, similar to many others used in the USEPA regulatory programs, to simulate environmental conditions to provide input for risk management decision-making. Both models present uncertainties (which are discussed in later sections and in TDM Documentation). However, we are confident that the outputs of these models adequately predict the PCB concentrations that are likely to result in abiotic and biotic media in the marine environment associated with the ex-ORISKANY artificial reef, and can be used reliably in the human health and ecological risk assessments for the ex-ORISKANY to support the Navy's pursuit of risk-based disposal approval for the vessel to be sunk for the creation of an artificial reef.

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This section describes PRAM's modules and governing equations by which they operate. It also details how the model algorithm works and points out its strengths and limitations. Modules discussed in this section are presented in Figure 3.

2.1 MODEL CONSTRUCT: BASIC CONCEPT

The PRAM is a "compartmental" or "box" model, that spatially and biologically defines an environment into which PCBs are released. Compartmental models consist of a number of interconnected compartments as Figure 4 shows. The arrows represent the PCB exchanges, or fluxes, that occur between the compartments. The initial source of PCBs within the system is from the sunken ship compartment (Compartment 5). The processes that control the fate and transport of the PCBs and modeling algorithms of those processes are discussed in Section 2.2.

The PRAM is also an "open system"[6] model where there is communication (exchange) with the environment that exists outside of the modeled environment (e.g., some material will leave the modeled environment due to a current flowing through the water compartments, a current flowing the air compartment, and possible sediment burial).

Each of the compartments within the modeled system are assumed to be homogeneously mixed, and to exchange chemical substances and energy following thermodynamic processes that can be described mathematically. Each compartment has a defined geometry, as well as a defined volume, density, and mass.

PRAM contains 11 categories of nonliving (abiotic) environmental compartments outside the sunken vessel (air, aerosols in air, epilimnetic water [upper water column], hypolimnetic water [lower water column], suspended solids in the upper and lower water columns, dissolved organic carbon in the upper and lower water columns, sediment on the ocean floor, sediment pore water, and dissolved organic carbon in pore water).

[6] Closed compartmental systems only interact with each other and are analogous to a closed bottle or jar containing a liquid and air space. PRAM is an open compartmental system where, for example, water flows into and out of the modeled environment and is analogous to water flowing through an open trough with its inlet and outlet.

Five basic assumptions are made for the exposure modeling[7] employed within PRAM (as adapted from Trapp and Matthies 1996):

1. The environmental compartments can be defined so as to represent phases or mixtures of phases in a thermodynamic sense (a phase is a physical stage of a chemical).
2. Rules and laws of chemical equilibrium and kinetics can be applied to describe PCB movement and/or fate.
3. Feedback of effects due to biota on PCB fate can be neglected.
4. Interactions among the various PCB homolog groups can be neglected, in the context of modeling PCB fate and transport.
5. Each PCB homolog series can be considered as a single phase in each compartment.

As pointed out by Trapp and Matthies (1996), these assumptions are not trivial. Regarding the first assumption, for example, "sediment" is actually a mixture of minerals, organic components, water, and biota. The simplifying assumption of using a single compartment for sediment in the model (instead of using several compartments to separately calculate changes in the mineral, organic, water, and biota fractions of sediment) represents a "general" level of resolution. A finer level of resolution could be achieved by adding more compartments within the sediment bed. However, as stated by Trapp and Matthies "*The model should only include the considerably important processes. It should also require a minimum of data and be comparable with environmental results*." Mackay et al. (1995) also addressed model complexity with the following statement: "*To select the appropriate model complexity, it is important to remember not to make the model more complex than the data set available…. Models should not be too complex, because it is then hard to obtain the data needed for calibration and validation.*" Thus, developing the PRAM requires an appropriate balance, or level of resolution, considering the complexity of the real-world environment it is attempting to characterize, but also the level of resolution in data that is available and/or obtainable to be used in PRAM, and the level of resolution needed in the PRAM outputs. The goal is to provide decision makers with additional information about the potential exposure conditions and human health risks associated with the ex-ORISKANY artificial reef so they can

[7] In the context here, exposure modeling refers to the estimation of PCB chemical concentrations in abiotic media to which biota (plants and animals) can be directly exposed.

determine whether the artificial reef would present an unacceptable risk to human health or the environment.

To keep the model minimally complex while being conservative, the PRAM was designed as a steady-state model. "Steady-state" in environmental modeling refers to the state where fluxes among compartments and across boundaries (i.e., between sources and sinks) are balanced, i.e., the concentrations of PCBs in various compartments remain the same as inflows to compartments balance outflows. The assumption of steady-state has a number of mathematical advantages in the context of risk assessments. These include, but are not limited to, the following:

- Within the mathematical algorithms, under an assumption of thermodynamic steady-state, the time-dependent differential terms for the algorithms can be set to zero, resulting in computationally easy solutions.
- A thermodynamic steady-state allows for the incorporation of empiric methods/results to define the highly complex interactions that result in environmental partitioning among various phases within the environment (e.g., it allows the use of empirically-derived partitioning coefficients such as K_{oc}, K_{doc}, K_{ow}, etc.).
- A thermodynamic steady-state represents the long-term overall condition of the system. This condition fits well with evaluations of chronic exposure regimes for potential receptors of concern (e.g., humans and long-lived ecologically relevant predators).

2.2 PHYSICAL AND CHEMICAL PROCESSES OF PCBS

Modeling the fate and transport of PCBs requires an understanding of those processes that functionally control or determine fate and transport ("forcing functions," see Mackay et al. 1995). Four physical processes/mechanisms are considered in PRAM: release, transport, partitioning, and transformation.

2.2.1 PCB Release from Shipboard Materials: Normalized Release Rates

Release, in environmental modeling represents the input of PCBs into the environment from bulk product materials within the vessel that contain PCBs. Within PRAM, PCB release is handled with an "empiric" method[8] (see Trapp and Matthies, 1996).

SSC-SD (2004) investigated, under laboratory conditions, the release of PCBs from a variety of PCB-containing bulk product materials that were collected from decommissioned US Navy vessels. The mechanisms that control PCB release from these shipboard materials are very complex, so no attempt was made to mathematically model the physicochemical processes. Instead, the observed empirical relationships between PCB releases, specific shipboard materials, and time were used for prospective modeling purposes (i.e., for the PRAM). These empirical observations (SSC-SD 2004) were made on those collected materials with the highest concentrations of PCBs observed from various sampling events. The resultant data are reported (SSC-SD 2004) in terms of the PCB homolog-specific release "rate," with units of nanogram of PCB per gram of PCB-containing material per day ($ng_{PCB}/g_{material}$-d).

The experiments used nine PCB-containing bulk product materials, seven of which were collected from ex-US Navy vessels: felt gaskets (2 types – inner and outer gasket material), rubber pipe hanger/liner material, bulkhead insulation, electrical cable, foam rubber material, aluminized paint, and standard samples of Aroclor© 1254, and Aroclor© 1268. Based on the leachate rate of PCBs from a known quantity of each material, the distribution of each homolog[9] series was determined and the release rates were adjusted to reflect release of the homolog series, as a total, on a per gram material per day basis (e.g., ng $_{monochlorobiphenyl}$ [$_{Mono-CB}$] / $g_{Material}$ – d). Additionally, a select subset of PCB congener masses per unit mass material per day was calculated (SSC-SD 2004).

Initial PCB releases from the shipboard materials occur quite rapidly, with an increase in rate followed by a decrease in rate over a longer period of time (see Figure 5).

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[8] The empiric method is generally applied for those systems and processes that are too complex or too little understood for a physicochemical mathematical description (modified definition from Trap and Matthies 1996, Mackay et al., 1995).

[9] As PCBs represent a mixture of 209 congeners that exhibit differences in environmental fate and effects, subsequent analysis utilized the grouping of the congeners by homolog series (the number of chlorines within the conger defines the homolog series or grouping, e.g., see Eisler and Belisle, 1996).

The varying release rates reveal a modeling approach issue, which is based on steady-state conditions within the system and in the context of the modeling objective (end product) – the chronic (30-year) reasonable maximum exposure level for humans consuming fish caught off the artificial reef. The leachate experiments show a significant decrease in release over the experimental period of approximately 18 months, equivalent to only about 5% of the chronic exposure period considered relevant for human health risk assessment (30 years). The general pattern of change within the data reported by SSC-SD (2004) reflects exponential decay after an initial period of increasing release. Integration of the release rates over a 30-year period is not possible using the existing data. To further characterize these data, they were statistically evaluated for the potential development of a functional relationship between homolog-specific release rate and time using regression analysis (Appendix A). This analysis was for only those data that represent detections[10] and was based on the natural log transformed PCB release rate in nanograms of PCB (by homolog) per gram of total PCB (sum total of all homologs) within the material per day (Appendix A). The reported rates from SSC-SD (2004) within the PRAM were normalized, by material, to the observed concentration of PCBs within the material used in the experimentation, prior to the statistical analysis.

The rationale for the adjustment of units is to account for the potential variation in PCB concentrations within materials collected from a ship being evaluated for disposal and those used in the laboratory measurements. This adjustment assumes that the relationship between release rate and PCB concentration is linear. For example, suppose that one vessel has 1,000 kilograms (kg) of an onboard material containing 100 milligrams (mg) of PCB per kg and the laboratory-observed release rate for this material is 1 nanogram (ng) PCB per gram (g) PCB per day. The total release (flux) from the material would be 100 ng PCB per day ([100 mg PCB/kg material * 1,000 kg material]/1,000 mg PCB/g PCB * 1 ng PCB/g PCB-day). Suppose another vessel, with the same 1,000 kg of onboard material contains a concentration of 50 mg PCB per kg. The total release or flux would be 50 ng PCB per day based on the 1 ng PCB per g PCB per day rate. Thus, by using the normalized release rates, variable material concentrations can be addressed.

The release rate regression format would be as follows, assuming exponential decay:

[10] As the objective of the statistical evaluation was to establish a functional relationship, it was believed appropriate to rely solely on detected and quantified values and not use surrogate values for non-detect samples that may skew or bias the statistical analysis.

(1) $$release\left[\frac{ngPCB}{gPCB}\right] = e^{a+b\cdot\ln(time)}$$

where:
release = PCB homolog series mass release per unit time
a = the intercept of the regression
b = the exponential slope of the regression
ln(time) = natural log of time

The decrease in release, based on those SSC-SD experimental data sets that could be regressed, is highly significant over a 30-year period. For example, the release rate of pentachlorobiphenyl from bulkhead insulation material peaks at 73 days after immersion into seawater. However, at 1 year the PCB release rate is predicted (based on the regression analysis) to be 37% of the peak rate; at 5 years to be 14% of the peak rate; and at 15 years and 30 years to be 7% and 4%, respectively, of the peak rate.

Not all of the leachate rate data sets (homolog series and material) revealed a statistically significant regression; some data sets contained only one or two detections for the homolog series while others contained only non-detects for the PCB homolog series.

Because PRAM is designed as a steady-state model, incorporating decay in the PCB release rate from the vessel is problematic. Modification to a TDM scheme to account for these release patterns was also considered problematic for the following reasons, among others:

- The existing data are insufficient to establish decay curves for all of the homolog series within the various PCB-containing shipboard materials.
- The approach would complicate the model; that is, other empiric approaches, for example, partitioning of the released PCBs into sediment, would no longer be appropriate.
- The resultant exposure levels would need to be integrated over time to calculate a reasonable maximum exposure level for human health risk calculations.

Thus, a constant release rate was considered appropriate for the model, if such a release rate was adequately conservative. It is anticipated that the colonization of an artificial reef will take a significant amount of time (e.g., 2 years). Additionally, the maximum bioaccumulation of PCBs, via the food web, into top predator fish (sports fish) taken for human consumption from the reef can require significant time for the heavier homolog groups (some much longer than 2 years). Therefore, a 2-year release rate was selected as a conservative *constant* release rate for modeling a steady-state condition. This rate is considered sufficiently conservative because it is treated as a constant (no decay over time) within the model, even though such a rate is much higher than the overall release rate over the exposure period assumed for risk characterization (30 years). For example, the predicted 2-year release rate for pentachlorobiphenyl from bulkhead insulation material is 5 times the predicted 30-year release rate.

When there were only one or two detections within the release rate data set (as obtained from SSC-SD 2004) or where the statistical analysis failed to produce a significant regression, the maximum reported rate was used in the PRAM. This is intentionally extremely conservative so as not to underestimate the overall resultant exposure levels to humans and relevant ecological receptors of concern.

The material-specific PCB homolog release rates incorporated into the PRAM are presented in Table 1.

2.2.2 Physical Transport Mechanisms

Diffusion, dispersion, and advection are the three physical "forcing functions"[11] within the PRAM. These three mechanisms drive the transport of PCBs within the modeled environment and are applied to the released PCBs within and outside the sunken vessel.

2.2.2.1 Diffusion

The molecules of a solute are in a state of continuous motion due to their kinetic energy. This motion, also called the Brownian motion, moves mass from regions of higher concentration (more molecules) to regions of lower concentration (less molecules). This gradual mixing or transport that occurs even in the absence of the bulk movement (advection) of fluid, is called "molecular diffusion." PCB molecules will show a net flux from places of higher concentrations to lower concentrations via molecular diffusion (e.g., see Trapp and Matthies, 1996). In one direction, diffusional flux is dependant on the area the

[11] Forcing functions are variables of an external nature that affect the state of the system (abbreviated definition from Mackay et al., 1995).

flux is occurring across, the thickness of the layer it is occurring across, and the concentration gradient (e.g., Trapp and Matthies, 1996; USEPA, 1982). The driving force for diffusion is the concentration gradient.

Diffusion is mathematically described by Fick's First Law, which assumes, (1) the medium within which it occurs and the direction in which it occurs remain constant, (2) the flux is perpendicular to the cross-sectional area of the boundary, and (3) the concentration gradient is constant (e.g., Trapp and Matthies, 1996; USEPA, 1982). Mathematically, molecular diffusion in one direction can be described as follows:

$$(2)\quad N_{diff\left[\frac{mol}{day}\right]} = A\left[m^2\right] \times \left(\frac{D\left[\frac{m^2}{day}\right]}{\Delta[m]} \times \left(C_2\left[\frac{mol}{m^3}\right] - C_1\left[\frac{mol}{m^3}\right] \right) \right)$$

where:
N = net substance flux due to diffusion (mol/day)
A = the surface area
D = the diffusion coefficient
$C_2 - C_1$ = the concentration gradient
Δ = the "thickness" of the diffusion gradient

Diffusion does not typically occur in a single direction in real situations, but in three directions simultaneously. Diffusion in the context of PCB transport within the environment is very slow compared to dispersion and advection. According to Lyman (1995), if advective water flow (i.e., current) is greater than 2×10^{-3} cm/s (4×10^{-5} knots), molecular diffusion can probably be ignored.

The importance of molecular diffusion within PRAM concerns "resistance" across media boundaries such as a pycnocline, surface water, and air interface, or the sediment bed – surface water interface (e.g., see Mackay et al., 1985; Mackay and Paterson, 1991; Trapp and Matthies, 1996). For this one-dimensional flux scenario Equation 2 (above) is appropriate. The quotient between the diffusion coefficient and diffusion length is termed "conductance" (mol/day), a measure of the exchange velocity and termed the "transport parameter" for exchange of PCBs across a boundary. The inverse of conductance is resistance, which can impede the partitioning of PCBs to sediments, for example, within a steady-state modeling scheme such as that used for the PRAM. This potential impedance is why diffusion is considered a relevant and important forcing function within the PRAM.

The area, concentration gradient, and thickness of the boundary are model variables within the PRAM whereas the diffusion coefficient is a chemical parameter. Mackay and Paterson (1991) present a single diffusion coefficient for hexa-CBs in water (4 x 10^{-4} m^2/hr), which was not considered appropriate as the PRAM attempts to model all ten PCB homolog series that differ among themselves regarding physicochemical properties, such as diffusion coefficients. Diffusion coefficients are proportional to temperature and inversely proportional to molar volume, which is related to the square root of the chemical molar mass (e.g., see USEPA, 1982; Trapp and Matthies, 1996), such that:

$$(3)\quad D_i / D_j = \frac{\sqrt{M_j}}{\sqrt{M_i}}$$

where:
D_i / D_j = the ratio between the diffusion coefficients for chemicals *i* and *j*
Mi and Mj = molar mass (g/mol) for chemicals *i* and *j*, respectively

This relationship leads to an estimation method that is functional for PCB homolog series. Using oxygen as a reference chemical, the diffusion coefficient in water, based on the mean molecular mass for each series, is estimated as follows (Baumgarten et al., 1996, USEPA, 1982):

$$(4)\quad D_{PCB-series} = 1.728 \times 10^{-4} \times \sqrt{\frac{32}{M_{PCB-series}}}$$

and for air (using steam as the reference chemical) is estimated as follows:

$$(5)\quad D_{PCB-series} = 2.22 \times \sqrt{\frac{18}{M_{PCB-series}}}$$

2.2.2.2 Dispersion

Molecular diffusion, in this context, occurs in perfectly quiescent media (water, air, sediment), which is rare in the environment. Turbulence occurs in open surface waters due to currents, in sediment beds via bioturbation by sediment-associated organisms and sheer stress from overlying water currents. Turbulent diffusion is the dominant forcing function in actual situations. Random turbulence (random physical movement in one or all directions) in the environment increases the apparent diffusion across physical boundaries such as those in the PRAM. Molecular diffusion, when supplemented by turbulence, is termed "dispersion"[12] (see Trapp and Matthies, 1996; USEPA, 1982). In effect, the additional physical movement to that of molecular diffusion leads into a greater velocity for the equilibration of chemical concentrations in space (i.e., increases the exchange velocity and thus impacts the transport parameter for exchange of PCBs across a physical boundary).

The physical movement component of dispersion differs from molecular diffusion; it almost always acts as a directional component associated with boundaries – for example, the water flow direction over a sediment bed where the turbulence is a consequence of the water current direction. Again, what is relevant for the PRAM is the exchange velocity of PCBs across the model boundaries where the velocities of media parallel to these boundaries (water-air, pycnocline, surface water-sediment bed) are much higher than the perpendicular exchange velocities across the boundary. In one dimension, dispersion can be described by the same equation (Equation 6) as that for molecular diffusion where:

$$(6)\quad N_{disp} = A\left[m^2\right] \times \left(\frac{D\left[\frac{m^2}{day}\right]}{\Delta[m]} \times \left(C_2\left[\frac{mol}{m^3}\right] - C_1\left[\frac{mol}{m^3}\right] \right) \right)$$

where:

N_{disp} = net substance flux due to dispersion (mol/day)

A = the surface area

D = the dispersion coefficient

$C_2 - C_1$ = the concentration gradient

Δ = the "thickness" of the boundary or diffusion gradient

However, D in Equation 6 is a "dispersion" coefficient, which is the sum of the diffusion coefficient as described in the previous "Diffusion" subsection, and that velocity (m^2/day) due to turbulence, which within the PRAM is a function of environmental setting and derived from empiric estimation techniques.

[12] In meteorology the term "eddy diffusion" is used.

2.2.2.3 Advection

By flowing movement of media such as water and/or air, PCBs contained within the media will be co-transported. This process is generally called "advection" (see Trapp and Matthies, 1996; Mackay et al., 1995; USEPA, 1982), although sometimes referred to as co-vection. Because volume and mass are conserved within each compartment of the PRAM, inputs of media (e.g., water) into a compartment must be balanced with output from the compartment either into another compartment or out of the model boundaries. The major advective flows within the PRAM include water current and air current. These currents are considered as overall averages since the PRAM is designed as a chronic exposure, steady-state model. Similarly, as long-term averages, these currents are considered to be unidirectional. Current within the sunken vessel is estimated based on the prevailing current within the surrounding water column, as a fraction of that current (e.g., 1%). Sunken vessels are known to "breathe" where water flows in and out of the open conduits. However, the PRAM assumes that, on average, there is a net advective flux of the PCBs from the interior of the vessel that is a consequence of the prevailing current exterior to the vessel.

The advection processes explicitly included in the PRAM are:

- Water currents that carry dissolved PCBs as well as PCBs absorbed onto suspended solids and PCBs bound to dissolved organic carbon within the water column.
- Air currents (wind) that carry PCBs that have volatized into the air column above the surface of the water.
- Wet and dry PCB deposits from the air column.

Implicitly included in the PRAM (i.e., processes included within the model algorithms) but assumed to be balanced (where input and output of PCBs is equal or net flux equals zero) are the advection processes for particulate deposition from the water column onto the sediment bed and resuspension from the sediment into the water column. This assumption results in no burial or sequestration of PCBs within the sediment bed, which is considered to be a conservative assumption.

2.2.3 Partitioning Coefficients

Within each of the PRAM compartments are "phases," which refer to the ability of the material to mix with another (e.g., since water and oil do not mix completely, each are considered a "phase"). At a thermodynamic steady-state, PCBs will exhibit predictable relative concentrations between phases or media. Given an adequate amount of time, the relative concentrations in water and organic carbon, for example, will reveal a constant ratio, regardless of the relative concentrations of PCBs in that water and organic carbon. The physicochemical processes associated with the phenomena are highly complex. As discussed above, the complexity of these "partitioning" processes is part of the rationale for the use of a steady-state modeling scheme instead of a TDM. These values have been measured and derived by numerous authors using various methods within the scientific literature. These partitioning coefficients have many sources, so a process was developed to select or derive the coefficients that are incorporated into the PRAM. The following paragraphs describe that selection process. Three partitioning coefficients are used within the PRAM, the octanol-to-water partitioning coefficient (K_{ow}), the water-to-particulate organic carbon partitioning coefficient (K_{oc}), and the water-to-dissolved organic carbon partitioning coefficient (K_{doc}). The following scheme was used to select or derive the coefficients that are incorporated into the PRAM:

- Measured values as reported in reputable (peer-reviewed) documents from regulatory agencies (i.e., USEPA, US Fish and Wildlife, Agency for Toxic Substances and Disease Registry [ATSDR], and scientific journals) were preferred,
- Empirically validated estimation methods obtained from reputable (peer-reviewed) documents from regulatory agencies were used when no measured values were obtained,
- Quantitative structure activity relationship (QSAR) estimation methods as described by reputable and/or regulatory agencies were used when no measured values or empirically validated estimation methods were obtained.

This approach is consistent with the approach used in USEPA's *Draft Dioxin Reassessment Documents* (USEPA, 2003). This reassessment included evaluation of dioxin-like compounds, which included PCB congeners. USEPA developed a ranking system to evaluate the degree of confidence in reported values of physical parameters (including partitioning coefficients) used in the reassessment. A property value with a ranking of one is considered to have the highest level of confidence. These ranks continue down to a ranking of five, which is the lowest level of confidence. The ranking scheme is based on the premise that measured values are more definitive than estimated values. USEPA specifically indicates that ranking five includes values derived by QSAR methods.

The octanol-to-water partitioning coefficients (K_{ow}) used within the PRAM are derived from the congener values presented within Eisler and Belisle (1996). Eisler and Belisle (1996) present the most complete set for PCBs based on a comprehensive review of data located within the peer-reviewed scientific literature. The congener values were subjected to statistical analysis to derive a mean value to represent each homolog group (Appendix B). Too few data are available for formal statistical analysis of the K_{ow} values for mono-CBs (3 values), nona-CBs (3 values), and deca-CB (single value). For both the mono-CB and nona-CB series, a simple average of the values presented by Eisler and Belisle (1996) was used. Deca-CB is represented by the value reported by Eisler and Belisle (1996). The derived homolog-specific K_{ow}s used in the PRAM are presented in Table 2.

The K_{oc} values used in the PRAM were derived in two ways. For the mono-CB through hexa-CB homolog series, K_{oc} measurements existed in the literature for congeners in these homolog series from which to calculate a K_{oc} value to use in the PRAM. For the PRAM, we select the K_{oc} values from Chou and Griffin (1986)[13] to calculate the representative K_{oc} values for each of these homolog groups. The K_{oc} values used for these homolog groups correspond to the geometric mean of the K_{oc} values measured for the individual congeners within an homologous series. Insufficient measurements of K_{oc} were found in the literature to allow determination of representative values for K_{oc} for the hepta- octa-CB, nona-CB and deca-CB homologous series. Therefore, a QSAR approach was taken to estimating these values. The equation used to estimate the K_{oc} is presented by Lyman (1995) and reproduced below:

$$(7)\quad \log_{10} K_{oc} = 0.779 \times \log_{10} K_{ow} + 0.46$$

The values for K_{ow} used in this calculation of K_{oc} for the hepta-, octa-, nona-, and deca-CBs are the geometric means of the K_{ow} values for all congeners within a given homologous series reported by Eisler and Belisle (1996) and are included on Table 2.

Partitioning of PCBs to dissolved organic carbon (K_{doc}) in water was related to the K_{ow} of the chemical by USEPA (2002). USEPA reported a ratio between K_{doc} and K_{ow} of 0.074 which is used to derive the K_{doc} for use in the PRAM. These derived K_{doc} values are presented in Table 2.

2.2.4 Transformation

PCBs, as xenobiotics, may be subject to certain enzymatically-mediated biotransformation processes to form metabolites, which may be different in physicochemical properties from the parent compounds (Kleinow and Goodrich, 1994).

Transformations of PCBs depend on the degree of chlorination; the more chlorinated forms are much more resistant to transformations than the lesser-chlorinated forms (Safe, 1990)[14]. Photolysis can occur for some forms in air and/or water, e.g., sunlight may react directly with many organic contaminants and dissolved organic carbon to produce photoreactant intermediates (Cooper, 1989). For PCBs, the importance of this transformation (dechlorination) is not suggested to be overly important in the context of PCB fate and transport mechanisms (ATSDR, 2000). Similarly hydrolysis and oxidation appear to be insignificant processes for PCB fate and transport (ATSDR, 2000).

PCB transformations mediated though biological processes (bio-degradation) are cited as the most important processes for PCB fate and transport in the environment (ATSDR, 2000). Table 3 presents a sampling of the reported biodegradation rates from the peer-reviewed scientific literature. Biodegradation rates for PCBs are highly variable among the congeners due to the degree of chlorination and structural characteristics of the PCB molecule. Variable biodegradation rates for the same congener are also expressed in the scientific literature, which has been linked to microbial pre-exposure to PCBs or other PCB-like compounds, bioavailability, microbial exposure concentrations, temperature, available nutrients, and the presence of inhibitory compounds (ATSDR, 2000).

[13] These data are reproduced in Appendix B.

[14] Safe (1990) showed that 2,4,5,2',4',5'-hexachlorinated biphenyl is recalcitrant to metabolism and very persistent in the environment. While with only 2 chlorines less than this compound, 3,4,3'4'-tetrachlorinated biphenyl is metabolized and less persistent in the environment. The net effect is that with time, both in the environment and in organisms, the predominant PCB congeners available for and contributed to bioaccumulation are those which resist degradation/transformation.

While biodegradation may be an important process for PCB fate and transport in the environment, this importance is limited to lesser-chlorinated forms and difficult to predict for any specific environmental setting such as that of an artificial reef. Therefore, within the PRAM, biodegradation is recognized and the model provides for rate inputs for each homolog series. However, to be conservative, the default condition of no biodegradation (or other transformation) is assumed to assure that the final exposure levels within the environment are not under-estimated. Residence time inside the vessel is considered too short for degradation inside the vessel to be significant.

2.3 SENSITIVITY ANALYSES

The purpose of a sensitivity analysis is to demonstrate a model's responses to alterations in uncertain input parameters. A sensitivity analysis provides the data necessary to rank the input parameters according to their influence on the model results. By ranking the parameters, one can identify those variables that require further investigation and define those variables to be used in an uncertainty analysis. Such a sensitivity analysis was performed on earlier versions of PRAM.

2.3.1 PRAM Version 1.1 Testing

Based on the sensitivity testing performed in 2001 on an earlier version of PRAM which predated the external peer review of the model, the parameters that were among the most sensitive for all types of fish were the following:

- $Log10K_{ow}$ (log of the octanol to water partitioning coefficient)
- $Log10K_{oc}$ (log of the organic carbon to water partitioning coefficient)
- Zone of influence - multiplier
- Sediment fraction organic carbon

Overall, the parameter groups that seemed to be the most sensitive were PCB inputs and environmental inputs.

2.3.2 PRAM Version 1.2 Testing

A more detailed sensitivity analysis was conducted for Version 1.2 of PRAM. PRAM Version 1.2 included refinements on several model variables, but the greatest improvement was the incorporation of additional exposure associated with the interior of the vessel. This version of PRAM contained 82 parameters:

- 18 human health exposure assumptions, oral reference doses, and cancer slope factors (Parameters 1 to 18 of the model);
- 17 bio-energetic inputs and dietary preferences for representative fish and shellfish species (Parameters 66 to 82 of the model); and
- 47 physical characteristics, PCB chemical properties, and biological characteristics (Parameters 19 to 65 of the model).

The first 18 parameters were not tested in the sensitivity analysis. A baseline PRAM scenario was designated as a benchmark. During the sensitivity analysis, each of the remaining parameters were varied from their respective baseline values one at a time over a range of values representative of the parameter. For each sensitivity scenario, the reasonable maximum exposure (RME) and central tendency exposure (CTE) for both cancer and non-cancer risks were calculated. This sensitivity analysis was conducted in a three-phased approach:

- **<u>Physical/Chemical Inputs</u>**. Sensitivity of calculated risk/hazard to each physical and chemical model input (Parameters 19 to 65) was evaluated in the first phase. Results were ranked for each species using a sensitivity coefficient:

$$S = \frac{|\partial R|}{(|\partial P| / P)}$$

where:

S is the normalized sensitivity coefficient which is a measure of the average change in the predicted variable per fraction change in the input variable. The higher the value of S, the more sensitive the input parameter.

∂R is the difference in the predicted risk between the base case and sensitivity case

∂P is the change in the input parameter between the base case and sensitivity case

P is the base input parameter value

Results were also evaluated based on a percent change in model-projected carcinogenic risk and non-carcinogenic hazard.

- **Bio-energetics/Food web.** Sensitivity of calculated risk/hazard to each bio-energetic input and dietary preference (Parameters 66 to 82) was evaluated in the second phase. These parameters consist of a series of dependent variables that had to be considered separately from the independent variables evaluated in the first phase. Results were evaluated for each type of fish using percent difference in projected carcinogenic risk or non-carcinogenic hazard:

$$PercentDifference = \frac{|\partial R|}{R}$$

where:
∂ R is the change in the risk from the base case to sensitivity case
R is the base model risk value

- **PCB-Laden Materials**. Sensitivity of calculated risk/hazard to changes in the amount of PCB-laden material on board the vessel was evaluated in the third phase. Both the amount of material and the PCB release rates for each type of material were evaluated. Results were evaluated using a percent difference ranking similar to that employed in the second phase.

The sensitivity analysis conducted on PRAM Version 1.2 qualitatively ranked the degree of impact on model results stemming from relatively equivalent variations in each of the parameters evaluated. The following parameters were identified as having the greatest impact on the PRAM-calculated risk/hazards:

- Zone of influence
- Partitioning coefficients Kow and Koc
- Fraction of organic carbon in sediment and suspended solids
- Active sediment depth
- Biodegradation rate constants (PRAM default is for no biodegradation)
- Release rate of PCBs from PCB-laden materials

The results from the sensitivity analysis conducted on PRAM Version 1.2 suggested a greater propensity to decrease rather than increase risk/hazard when looking at the range of potential inputs. This indicates that reasonably conservative default values are incorporated into the baseline case of the model. However, it is also important to note that multiple organisms in the food chain are each affected by variables associated with both bio-energetics and dietary preferences. Some additivity among food chain components may occur, particularly to higher trophic level species. Potential additivity was not represented in the PRAM Version 1.2 sensitivity analysis.

The analysis concerning the amount of PCB-containing material indicates a link to the release rate of the material. If the individual amount of material is changed, the risk is affected by a percentage directly related to the release rate. The greatest change in risk/hazards stemming from PCB-containing materials involved felt gasket material.

2.3.3 PRAM Version 1.4c Testing

PRAM Version 1.4c is an enhanced version of PRAM Version 1.2. Several significant enhancements have been made to the model; however, the basic governing equations within the model itself have not changed. Therefore, knowledge gained from the extensive sensitivity analysis testing performed on previous versions of PRAM has been used to design the sensitivity analysis testing program for PRAM Version 1.4c. Two categories of input parameters were considered for the PRAM Version 1.4c sensitivity analysis:

- **Abiotic Inputs**. This category includes the physical/chemical inputs and the PCB-laden materials factors that were evaluated during the PRAM Version 1.2 sensitivity analyses.
- **Bio-energetics/Food web**. This category includes the same biological parameters that were evaluated during the PRAM Version 1.2 sensitivity analyses.

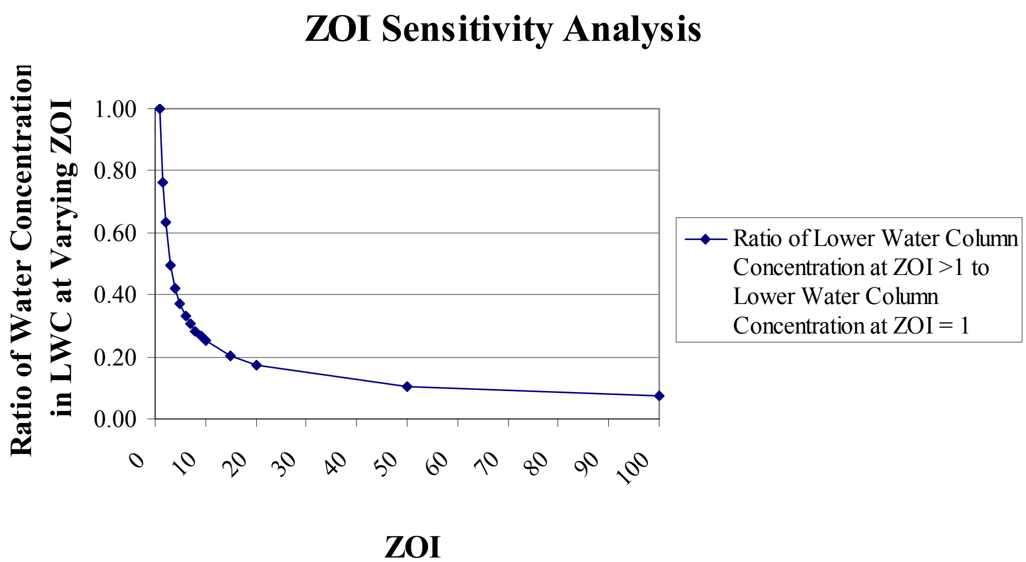
Abiotic Sensitivity Analysis

Variations in the abiotic input parameters in PRAM Version 1.4c are expected to produce relatively similar changes in model results as occurred during the sensitivity analyses of the earlier versions of PRAM, particularly Version 1.2. Given that variation in most abiotic parameters decreased, rather than increased, the risk/hazard in PRAM Version 1.2, the sensitivity analysis for PRAM Version 1.4c focused on the model parameter that exerted the greatest effect on the PCB concentrations in the water, the Zone of Influence (ZOI). The

ZOI was identified as the parameter having the greatest impact on model results in the sensitivity analyses conducted for PRAM Version 1.2 and one of the highest for PRAM Version 1.1. Also, selecting the ZOI is probably the most subjective parameter input entered into the PRAM because the ZOI artificially establishes limits within which PCB concentrations are presumed to affect the biota. For these reasons, the sensitivity analysis for abiotic parameters was limited to the ZOI.

The concept of the ZOI is explained graphically in Figure 13. The ZOI represents a volume established by extending the area of a horizontal ellipse vertically through the various layers or columns – sediment, lower water column, upper water column, and air – where the model results will be calculated. The vessel emitting the PCBs is centered within this horizontal ellipse resting on top of the sediment at the bottom of the lower water column (LWC). The resulting volume of the elliptical cylinder is determined by the area of the horizontal ellipse. The minimum volume ZOI is determined by applying the "footprint" or area of the vessel, assuming it is resting upright on the sea floor. Therefore, the minimum ZOI, or ZOI = 1, represents an ellipse with the area created by multiplying the length and the width of the vessel. The minimum ZOI must encompass the maximum horizontal area of the vessel for all of the PCB source to be included within the ZOI. Larger ZOI designations are referenced to the number of multiples of the maximum horizontal area of the vessel included within the ellipse forming the elliptical cylinder. Therefore, a ZOI = 2 means that the area of the horizontal ellipse forming the elliptical cylinder is twice the maximum horizontal vessel area; ZOI = 3 means the area is three times the vessel area; etc. The axes of the horizontal ellipse are expanded equally to produce the larger areas as the ZOI expands as shown in Figure 13.

As the ZOI expands, the resulting PCB concentrations in the various columns decline because the mass entering the system from the source (the vessel) remains constant while the volume of the elliptical cylinder increases. The impact on PCB concentrations of varying the ZOI is displayed in the following graph.



The horizontal or x-axis represents the ZOI increasing from a value of 1 which represents the minimum ZOI. The vertical or y-axis represents the ratio of the PCB concentration in the LWC at the given ZOI value divided by the maximum PCB concentration in the LWC that occurs when the ZOI = 1. The ratio represents the fractional amount of the original PCB concentration remaining as the ZOI increases. Subtracting the ratio from one provides the fractional amount that the original PCB concentration has decreased as the ZOI increases. The applicable percentages can be determined by multiplying the respective fractions by 100.

As displayed in the graph, most of the reduction in PCB concentrations occurs when the ZOI expands from 1 to 10, then the rate of PCB concentration reduction diminishes significantly as the ZOI increases to 100. At a ZOI = 1.5, the resulting ratio is approximately 0.76 indicating the original PCB concentration has decreased by about 24% when the base of the ZOI has been expanded by just 50%. When the ZOI = 3, the ratio is close to 0.50 showing that approximately 50% of the original PCB concentration is eliminated by expanding the base of the ZOI to encompass three times the maximum horizontal area of the vessel.

Bio-energetics/Food web Sensitivity Analysis

Five parameters involving bio-energetics and/or food web considerations were examined during the biological sensitivity analysis. These five parameters include:

- Octanol to water partition coefficient, K_{ow};
- Respiration rate regression parameter β2;
- Depuration rate, Ke;
- Growth rate, G; and
- Assimilation efficiency, α.

The octanol to water partition coefficient was identified as one of the parameters having great impact on the PRAM-calculated risks/hazards during sensitivity analyses of the earlier versions of PRAM. The respiration rate was investigated because it directly influences the degree to which aquatic organisms take up PCB constituents from other than dietary sources. The depuration rate and the growth rate were selected for sensitivity analyses because of their significant impact on the Biological Concentration Factor (BCF). The BCF represents the tendency of species to take up PCB constituents from factors other than diet. Similarly, the assimilation efficiency was chosen for sensitivity analysis due to its influence on the Biological Accumulation Factor (BAF). The BAF represents the tendency of species to take up PCB constituents from all sources, including diet.

Octanol to water partition coefficient, K_{ow}. The K_{ow} represents the affinity PCB constituents have for entering lipids (fat tissue) in preference to remaining dissolved in water. The higher the K_{ow} is, the more PCB constituents tend to be taken up by biota rather than remaining dissolved in the surrounding water. Each PCB homolog group has a specific K_{ow} value as indicated in Table 2. A sensitivity analysis was conducted by varying the K_{ow} from the base case (K_{ow} x 1) by decreasing the value to half the base case (K_{ow} x 0.5) and also by doubling the value (K_{ow} x 2). The resulting percent difference in Central Tendency Exposure (CTE) risk from the base case was determined. The percent differences for cancer risk and non-cancer hazard were the same for the species included in the sensitivity analysis. The results for this sensitivity analysis are shown in the following chart:

CTE RISK ESTIMATES Species	K_{ow} x 0.5 Percent Difference	K_{ow} x 2 Percent Difference
Benthic fish TL-IV (flounder)	-22.97	+10.64
Benthic shellfish TL-III (lobster)	-7.39	+3.78
Pelagic fish TL-IV (jack)	-33.12	+25.78
Reef fish TL-IV (grouper)	-43.12	+43.16
Reef fish TL-III (triggerfish)	-27.62	+17.83
Reef shellfish TL-III (crab)	-12.72	+1.85

As depicted in the chart, reducing the K_{ow} values to half the base case values for the species represented reduced the resulting PCB risks/hazards by 7% to 43%. Similarly, doubling the K_{ow} values from the base case increased the resulting PCB risks/hazards by 2% to 43%. Considering that the higher trophic levels (TL-IV) tend to consume the lower trophic levels (TL-III), particularly within a specific community of biota (benthic, pelagic, or reef), the percent differences in risks stemming from variations in the K_{ow} values generally are larger in the higher trophic species.

Respiration rate regression parameter, β2. The respiration rate represents the amount of oxygen taken up by a particular aquatic species per mass of lipids content within a single day. The respiration rate for a given species is determined by regression analysis on laboratory measurements of actual oxygen consumption. Depending on the species, this regression analysis yields either two or three coefficients that can be used with an exponential equation to estimate the respiration rate for the species as a function of temperature. Of these coefficients, the parameter designated as β2 has the most significant impact on the calculation because it is multiplied by the exponential term in the equation. Therefore, the higher the value of β2 is, the higher the respiration rate is for that particular species at a given temperature. As the respiration rate increases, the amount of PCBs taken up by the aquatic organism also increases. A sensitivity analysis was conducted by varying the β2 value from the base case (β2 x 1) by decreasing the value to half the base case (β2 x 0.5) and also by doubling the value (β2 x 2). The resulting percent difference in CTE risk from the base case was determined. The percent differences for cancer risk and non-cancer hazard were the same for the species included in the sensitivity analysis. The results for this sensitivity analysis are shown in the following chart:

CTE RISK ESTIMATES Species	β2 x 0.5 Percent Difference	β2 x 2 Percent Difference
Benthic fish TL-IV (flounder)	-31.06	+55.39
Benthic shellfish TL-III (lobster)	-20.01	+25.46
Pelagic fish TL-IV (jack)	-58.40	+149.36
Reef fish TL-IV (grouper)	-40.99	+140.67
Reef fish TL-III (triggerfish)	-25.44	+66.58
Reef shellfish TL-III (crab)	-28.71	+55.44

As depicted in the chart, reducing the β2 values to half the base case values for the species represented decreased the resulting PCB risks/hazards by 20% to 58%. Similarly, doubling the β2 values from the base case increased the resulting PCB risks/hazards by 25% to 149%.

Considering that the higher trophic levels (TL-IV) tend to consume the lower trophic levels (TL-III), particularly within a specific community of biota (benthic, pelagic, or reef), the percent differences in risks stemming from variations in the β2 values generally are larger in the higher trophic species.

The corresponding respiration rates (gO2/kg_lipid-day) varied from -45% to -76% when β2 values were reduced to half the base case values. When β2 values were doubled from the base case, the resulting respiration rates varied from +229% to +1,689%.

Depuration rate, Ke. The depuration rate represents the rate at which PCB constituents entering an aquatic species are eliminated from the biota rather than taken up in lipids or fat tissue. The higher the depuration rate is, the lower the BCF is for that particular species, and the resulting PCB concentrations in the biota are lower. A sensitivity analysis was conducted by varying the depuration rate from the base case (Depuration x 1) by decreasing the value to half the base case (Depuration x 0.5) and also by doubling the value (Depuration x 2). The resulting percent difference in CTE risk from the base case was determined. The percent differences for cancer risk and non-cancer hazard were the same for the species included in the sensitivity analysis. The results for this sensitivity analysis are shown in the following chart:

CTE RISK ESTIMATES **Species**	**Depuration x 0.5** **Percent Difference**	**Depuration x 2** **Percent Difference**
Benthic fish TL-IV (flounder)	+35.93	-34.42
Benthic shellfish TL-III (lobster)	+16.55	-19.62
Pelagic fish TL-IV (jack)	+57.05	-43.35
Reef fish TL-IV (grouper)	+76.10	-51.95
Reef fish TL-III (triggerfish)	+44.63	-38.84
Reef shellfish TL-III (crab)	+27.49	-27.21

As depicted in the chart, reducing the depuration rates to half the base case values for the species represented increased the resulting PCB risks/hazards by 17% to 76%. Similarly, doubling the depuration rates from the base case decreased the resulting PCB risks/hazards by 20% to 52%. Considering that the higher trophic levels (TL-IV) tend to consume the lower trophic levels (TL-III), particularly within a specific community of biota (benthic, pelagic, or reef), the percent differences in risks stemming from variations in the depuration rates generally are larger in the higher trophic species.

The corresponding water BCF values varied from +1% to +16% when depuration rates were reduced to half the base case values. When depuration rates were doubled from the base case, the resulting water BCF values varied from -2% to -22%.

Growth rate, G. The growth rate is the rate at which aquatic species increase in mass as they age. The higher the growth rate is, the lower the BCF is for that particular species, and the resulting PCB concentrations in the biota are lower. A sensitivity analysis was conducted by varying the growth rate from the base case (Growth x 1) by decreasing the value to half the base case (Growth x 0.5) and also by doubling the value (Growth x 2). The resulting percent difference in CTE risk from the base case was determined. The percent differences for cancer risk and non-cancer hazard were the same for the species included in the sensitivity analysis. The results for this sensitivity analysis are shown in the following chart:

CTE RISK ESTIMATES Species	Growth x 0.5 Percent Difference	Growth x 2 Percent Difference
Benthic fish TL-IV (flounder)	+526.38	-77.75
Benthic shellfish TL-III (lobster)	+302.09	-66.45
Pelagic fish TL-IV (jack)	+294.56	-73.17
Reef fish TL-IV (grouper)	+302.33	-72.47
Reef fish TL-III (triggerfish)	+206.50	-66.04
Reef shellfish TL-III (crab)	+124.20	-56.53

As depicted in the chart, reducing the growth rates to half the base case values for the species represented increased the resulting PCB risks/hazards by 124% to 526%. Similarly, doubling the growth rates from the base case decreased the resulting PCB risks/hazards by 57% to 78%. Considering that the higher trophic levels (TL-IV) tend to consume the lower trophic levels (TL-III), particularly within a specific community of biota (benthic, pelagic, or reef), the percent differences in risks stemming from variations in the growth rates generally are larger in the higher trophic species.

The corresponding water BCF values varied from +57% to +96% when growth rates were reduced to half the base case values. When growth rates were doubled from the base case, the resulting water BCF values varied from -42% to -49%.

Assimilation efficiency. The assimilation efficiency represents the degree to which various species take up PCB constituents from their diets. As the assimilation efficiency increases, the more PCB constituents magnify in the food chain. This results in higher PCB concentrations in higher trophic species. The base case represented close to the maximum assimilation efficiency that could be expected for the species represented. Some of the species could not have their assimilation values doubled without exceeding 100%. Therefore, a sensitivity analysis was conducted by decreasing the assimilation efficiency first by 50% (Assimilation x 0.5) from the base case (Assimilation x 1) and then by 75% (Assimilation x 0.25). The resulting percent difference in CTE risk from the base case was determined. The percent differences for cancer risk and non-cancer hazard were the same for the species included in the sensitivity analysis. The results for this sensitivity analysis are shown in the following chart:

CTE RISK ESTIMATES **Species**	**Assimilation x 0.5** **Percent Difference**	**Assimilation x 0.25** **Percent Difference**
Benthic fish TL-IV (flounder)	-67.65	-84.22
Benthic shellfish TL-III (lobster)	-42.83	-56.45
Pelagic fish TL-IV (jack)	-69.33	-84.92
Reef fish TL-IV (grouper)	-66.23	-81.68
Reef fish TL-III (triggerfish)	-51.04	-68.76
Reef shellfish TL-III (crab)	-29.80	-44.48

As depicted in the chart, reducing the assimilation efficiencies to half the base case values for the species represented decreased the resulting PCB risks/hazards by 30% to 69%. Similarly, decreasing the assimilation efficiencies to 25% of the base case decreased the resulting PCB risks/hazards by 44% to 85%. Considering that the higher trophic levels (TL-IV) tend to consume the lower trophic levels (TL-III), particularly within a specific community of biota (benthic, pelagic, or reef), the percent differences in risks stemming from variations in the assimilation efficiencies generally are larger in the higher trophic species.

The corresponding BAF values varied from -33% to -80% when assimilation efficiencies were reduced to half the base case values. When assimilation efficiencies were to a quarter of the base case, the resulting BAF values varied from -49% to -93% of the corresponding species base case BAF values.

2.4 MODEL UNCERTAINTIES AND LIMITATIONS

In environmental risk management, the confidence in a model, such as PRAM, to provide useful input for decision-making will increase if the model has certain attributes. These attributes may include: that the model follows USEPA guidance; has been peer reviewed;

and has incorporated peer-reviewed and/or scientifically valid algorithms, and site-specific input, and that any conservatism incorporated into the model is reasonable and plausible. The Navy has pursued these goals in the design and construction of PRAM. Moreover, a model is limited by the variables that we can account for, and the possibility that a significant variable has been missed or misrepresented. In developing the PRAM, all variables believed relevant and applicable have been incorporated, to the best of the ability of the modelers and Navy contractors. Nevertheless, the PRAM is limited by some attributes that have been incorporated as improvements and others that are intrinsic to all models and computer simulations.

2.4.1 Strength

The PRAM, as with any computer simulation, is limited by the quality and quantity of information upon which the predicted outcomes are based. The site-specific information provided by the Navy and its contractors concerning the type and mass of PCB-containing materials, and by the State of Florida and Escambia County concerning the environmental setting for the ex-ORISKANY, should be considered a strength for the predictions made here.

More generally, the PRAM contains a significant number of attributes that can be considered strengths:

- Leach rates data based on experiments that simulated the environment (temperature, pressure, and salinity), in which leaching of PCB from the product materials in seawater is expected to take place.
- Algorithms used for predicting the fate and transport of PCBs in the aquatic environment are well established and generally accepted by the scientific community (e.g., same basic algorithms as those used by the USEPA in the development of the PCB water quality standard for the Great Lakes).
- PCBs are modeled as homologs or groups of PCBs with similar physical, chemical, and biouptake/bioaccumulation properties, resolving the difficult issue of assessing the impacts of PCBs as a mixture in the products.
- The ability to address various classes of ships with variable amounts and types of PCB-containing bulk product materials onboard with variable PCB concentrations.

- The ability to make scenario analysis to ascertain risk-reduction benefits from a hypothetical level of mitigation of PCB-containing bulk product material.
- The design of PRAM is based on consensus reached among scientists in the TWG, resolving such issues as ZOI (horizontal and verticality extent), and diet-water compositions for various relevant species in different trophic levels.
- Relatively easy to use with the help of the GUI, and can be used to support the assessment of risks during the “transient” or pulse-release period.

The model has been checked for mathematical correctness, structure, and underlying premises. In addition to the USEPA, the Navy is also requesting review and comment from its independent reviewer, RTI.

The greatest strength of the PRAM is its capability to serve as a predictive model or tool to assist in the decision-making process associated with the use of decommissioned Navy vessels as artificial reef building material.

2.4.2 Limitations

“All models are wrong, but some are useful” is a common saying within the fate and transport and risk modeling community. This observation is appropriate in emphasizing to risk managers that a model is a tool for decision-making. While models attempt to predict or mimic reality based on scientific principles and built-in assumptions and conservatism, it is, in and of itself, not a faultless predictive tool. Uncertainties or limitations of PRAM include:

- The PRAM requires boundaries for the modeled environment (i.e., the PRAM models an “oval-shaped column” around the sunken vessel within the ocean – as based on the ZOI). The ZOI dimensions, albeit based on TWG consensus and scientific justifications (Appendix F), are best-guessed conservative estimates.
- The vessel is assumed and modeled as a porous material where the PCBs are moving from the interior to the exterior uniformly around the reef established on the ship.
- The PRAM assumes steady-state conditions are present.

- The PRAM does not account for the importation of water or suspended sediment containing PCBs from outside the system being modeled.
- The PRAM does not account for variable life histories of the animals within the system whereas some fish may have accumulated PCBs from juvenile rearing in ports and bays.
- The food web module in PRAM is not intended to be all encompassing; although it is based on consensus within the TWG, only significant and relevant or representative species in the food web pathway are included for biouptake/bioaccumulation.
- The PRAM has not been calibrated with empirical data, has not been updated to perform probabilistic risks to assess uncertainties, and has not been upgraded to perform multiple sunken vessel risk modeling.[15]

Uncertainties are always associated with exposure scenario and parametric variability in risk assessment modeling. Overall, PRAM is considered a useful risk management tool for the Navy REEFEX program because the program follows USEPA risk assessment methodology, uses algorithms and structure accepted by the scientific community, has been validated (i.e., they were used successfully in previous applications [e.g., Connolly, 1991; USEPA, 1995]), and has undergone independent review. PRAM could be further improved, to reduce uncertainty, by calibration against empirical data.

2.5 ABIOTIC MODEL SELECTION OF PCB FATE AND TRANSPORT

Fugacity modeling has been used in multimedia applications and has received a great deal of attention for use in environmental decision-making (Cowan et al., 1995). For example, the California Environmental Protection Agency (Cal/EPA) has developed an Excel®-based

[15] Calibration against actual data (e.g., PCB concentrations in marine organisms within selected tropic levels) should help improve model accuracy and/or confidence in the model. Calibration could be achieved by adjusting bioenergetic algorithms, e.g., gastrointestinal absorption efficiency. Performance of probabilistic risk simulations is a requirement per EPA guidance to present a full-spectrum of risks, not just high-end and central tendency risks. Performance of a multiple sunken-vessel scenario would be needed if there is a plausible need to perform such risk calculations (e.g., a cluster of sunken vessels documented or purported to have PCB-containing materials is to be sunk at a specific locality). In addition, if PRAM is to be used to estimate ecological risks for comparison with benchmark values, incorporation of a more representative food web would be necessary. PRAM could also be improved to assess the risk-reduction impact of various remedial options, particularly to address the uncertainty associated with PCB-containing materials that have bi-modal or non-normally distributed data.

Level III fugacity model to assist in assessing contaminated sites within the state (CalTOX, UC-Davis [UCD] and Lawrence Livermore National Laboratory [LLNL], 1994; McKone et al., 1997). A Level III fugacity approach was used in developing the ambient water criteria for the Great Lakes Water Quality Initiative (USEPA, 1995; Gobas, 1993). ChemCAN is also a Level III fugacity model, developed for Health Canada to assist in evaluating regional pollutant issues within Canada. HAZCHEM was developed for European Union Member States as a Level III fugacity model (European Centre for Ecotoxicology and Toxicology of Chemicals [ECETOC], 1994) for examining and evaluating pollutant risks.

In the Navy's judgment, fugacity-modeling approaches are appropriate and defensible given their wide use and acceptance by the regulatory community. Thus, the PRAM employs the fugacity modeling approach.

What follows is a general description of the various fugacity modeling "levels" and the specific structure of the PRAM fugacity module that is based on the Level III fugacity construct.[16]

2.5.1 The Fugacity Multimedia Approach

Fugacity (*f*) is the "escaping tendency" of a chemical from a particular phase (Mackay and Paterson, 1981) with units of pressure (Pascals [Pa]). This fugacity can be related to the phase (e.g. environmental media) physically as the partial pressure or "escaping" potential exerted by a chemical in one compartment (physical phase such as water, sediment, air) on another. When a chemical is at equilibrium between two phases, the escaping tendency or "fugacity," of the chemical is the same for the two phases (i.e., a common fugacity among media). This represents an extension of partitioning theory.

In the scientific literature, the four "levels" of fugacity modeling are:

- Level I – a closed system at equilibrium (common fugacity) and at thermodynamic steady-state, with no chemical reactions.

[16] Version 1.3 of the PRAM used a level II fugacity modeling approach, while Version 1.4c of PRAM uses a level III fugacity modeling approach.

- Level II – an open system at equilibrium (common fugacity), and at thermodynamic steady-state, with chemical reactions.
- Level III – an open system not at equilibrium (no common fugacity, except within compartments) while at thermodynamic steady-state, with chemical reactions.
- Level IV – an open system not at equilibrium (no common fugacity, except within compartments) and not at thermodynamic steady-state, with chemical reactions.

2.5.1.1 Model I Fugacity Model

Level I fugacity model represents a closed system at equilibrium (or common fugacity) that is at thermodynamic steady-state, with no chemical reactions occurring within the system. A closed system is akin to a closed jar containing chemical and media (e.g., water, sediment, air). No inputs or outputs occur within the system aside from the starting conditions; a Level I fugacity model predicts the distribution of the chemical within these media at equilibrium, under steady-state conditions. This model, when used for a system that has only two media or phases (such as organic carbon and water), will result in a partition coefficient that is equal to the K_{oc} as described previously, albeit derived differently. Using the fugacity concept and a common fugacity (*f*), which assumes equilibrium, this situation can be expressed mathematically as:

$$\frac{C_i}{C_j} = \frac{fZ_i}{fZ_j} = \frac{Z_i}{Z_j} = K_{ij}$$

Where C is the concentration of the chemical (mol/m^3) in phase *i* or *j*, *f* is the common fugacity (Pa), Z is the fugacity "capacity" of phase *i* or *j*, with units of (mols /m^3 * Pa), and K_{ij} equals the partitioning coefficient for the chemical and the respective phases of *i* and *j*. (see also Equation 17). Using fugacity capacities, the partitioning of multiple phases within the system is highly simplified. Consider, for example (per Mackay and Paterson, 1981), a 10-phase system in which potentially 90 partitioning coefficients may be defined independently (e.g., K_{oc}). As the ratios of the fugacity capacities are equivalent to the partition coefficients, the solution can be obtained with far greater ease. The dissection of equilibrium constants into individual fugacity capacities is a convenient method that facilitates calculation of a chemical's quantities via partitioning within variable multi-media systems regardless of whether it is a closed or open system.

The fugacity capacity for vapors, as discussed by Mackay and Paterson (1981), assuming standard atmospheric pressure, can be related back to the partial pressure and the ideal gas law. Thus, Z for air is represented as:

(8) $$Z_{air} = 1/(R \times T)$$

where:
R = Universal Gas Constant (8.31 Joules/mol-°K)
T = temperature (°K)

Particulate matter within the air column are considered to be aerosols (per Mackay and Paterson, 1991) with a fugacity capacity of:

(9) $$Z_{aerosols} = 6 \times 10^{6} / (VP \times R \times T)$$

where:
VP = liquid vapor pressure (Pa)
R = Universal Gas Constant (8.31 Joules/mol-°K)
T = temperature (°K)
6×10^6 = a constant as derived by Mackay and Paterson (1991) (Pa)

Vapor pressures for individual PCB congeners were obtained from Fiedler, 2001; Oberg, 2001; and the ATSDR Toxicological Profile for PCBs, 2000. Where possible (i.e., sufficient number of values) statistical analysis was performed to derive a homolog-specific vapor pressure (Appendix C). The vapor pressures used in the PRAM are presented in Table 2.

The fugacity capacity for water (as a pure phase), assuming a non-ionizable molecule (like PCBs), and invoking "infinite dilution" (see Mackay and Paterson, 1981), reduces to the reciprocal of the chemical's Henry's Law Constant (Pa – m^3/mol).

(10) $$Z_{water} = 1/H$$

Freshwater solubility is necessary to estimate the Henry's Law Constant per Mackay and Paterson (1981, 1991). Solubility of PCBs in freshwater were obtained from Chou and Griffin (1986). When solubility data were unavailable, the following estimation method presented by Lyman (1995) was used:

$$(11)\quad \log S\left[\frac{mol}{L}\right] = -1.16 \times \log K_{OW} + 0.79$$

This equation was used to estimate the water solubility of octa-CB, nona-CB, and deca-CB. The solubility values used within the PRAM are presented in Table 2.

The vapor pressures and solubilities for the respective PCB homolog series were used to estimate the Henry's Law Constant (H) per equation 21 within Lyman (1995):

$$(12)\quad H\left[\frac{Pa \cdot m^3}{mol}\right] = \frac{VP[Pa]}{S\left[{}^{mol}\!/_{m^3}\right]}$$

The Henry's Law Constant values for each PCB homolog series as used within the PRAM are presented in Table 2.

As pointed out above, partitioning coefficients can be related to the ratio of chemical fugacity capacities (for sorbed phases such as sediment, total suspended solids), and dissolved organic carbon (Mackay and Paterson, 1981, 1991):

$$(13)\quad Z_{TSS} = \frac{(K_{oc} \times f_{oc-TSS}) \times \rho_{TSS}}{H}$$

$$(14)\quad Z_{\text{sediment}} = \frac{(K_{oc} \times f_{\text{oc-sediment}}) \times \rho_{\text{sediment}}}{H}$$

$$(15)\quad Z_{DOC} = \frac{K_{DOC} \times \rho_{DOC}}{H}$$

where:

TSS = total suspended solids

DOC = dissolved organic carbon
H = Henry's Constant (Pa –m^3/mol)
K_{oc} = the organic carbon to water partitioning coefficient for PCBs (L/kg-oc)
K_{DOC} = the dissolved organic carbon to water partitioning coefficient for PCBs (L/kg-DOC)
$f_{oc\text{-}TSS}$ or sediment = the fraction of organic carbon within the suspended solids or sediment (unitness)
ρ_{media} (TSS, sediment, or DOC) = bulk density of the media (g/cm^3)

Using these fugacity capacities, partitioning within a system containing air, water, sediment, total suspended solids, and dissolved organic carbon can be predicted with a minimal amount of data requirements. This partitioning is relative in concentration such that volumes and mass are required to solve for absolute concentrations, which is derived from the total mass of chemical present and a common fugacity where:

$$(16)\quad f = \frac{M_T}{\sum Z_i V_i}$$

Where f is the common fugacity (equilibrium), M_T is the total mass (mols) introduced into the closed system, Z_i is the fugacity capacity for system phase or compartment i, and V_i is the volume of the phase in m^3. The relationship between fugacity, fugacity capacity and chemical concentration (C in mols/m^3) is defined by:

$$(17)\quad C = Zf$$

The Level I fugacity model assumes no input and/or output of media or chemical and is useful in describing simple partitioning problems but not adequate for modeling PCBs being released from a sunken vessel because: (1) the sunken vessel is an open system, (2) no common fugacity occurs within the system except within compartments, and (3) chemical reactions may occur within the compartment (such as dechlorination/degradation). It is, however, illustrative of the basic underpinnings of the fugacity concept and escaping tendency.

2.5.1.2 Model II Fugacity Model

Very few closed systems exist in the environment whereby there are no exchanges with the outside of the model construct (outside of the model boundaries). Although a Level I model is useful to assess relative distributions of a chemical in a closed system, it is not applicable to environmental systems such as the sunken vessel environment for the PRAM. This is due to water current and the lack of a physical boundary that keeps the PCBs from moving further away from the vessel. Level II fugacity models, like Level I models, assume system equilibrium and steady conditions. However, they are used to represent "open" systems where inputs to and outputs from the system compartments are included. This type of system has a chemical input into the system (e.g., emission or release), which is balanced by the system media trapping the chemical, reactive losses, and chemical output from the system. Thus, all of the inputs to and losses from the system are balanced (steady-state) as well as exchanges between the compartments (equilibrium). The Level II model is simplistic because it assumes a common fugacity (equilibrium) such that the exchanges between the compartments (e.g., water and sediment) are not subject to any transfer resistances. The advantage of this system is limited data requirements and a simple algebraic solution. The driving forces within such a system are limited to fate and transport between compartments, i.e., advection and chemical reactions in the sunken vessel environment. Advection in and out of the system compartments can be introduced into the Level II model as a first-order constant; as advective flow with units of m^3/day divided by the phase volume, e.g., water (V in m^3) with resultant units of 1/day. Additionally, other rate constants for reactive processes such as dechlorination/degradation can be included. By assuming equilibrium among compartment (phases) and steady-state conditions where input, output, and transfers among phases are balanced, a common fugacity can be calculated based on emission (mol/day) into the system (Mackay and Paterson, 1981):

$$(18) \quad f = \frac{N}{\sum V_i Z_i K_i}$$

Where, as in the Level I fugacity model, f is the common fugacity, N is the mass emission (mols/day) introduced into the system, Z is the fugacity capacity for the system phase or compartment i, V_i is the volume of the phase in m^3, and K_i is the first-order rate for advection and any additional reactive rate constant occurring within the respective phase or compartment.

This equation can be rewritten to explicitly describe rates and transport using a D value to more explicitly represent transport mechanisms (Mackay and Paterson, 1991; Mackay et al., 1995):

$$(19) \quad N = f\left(\sum D_{Ai} + \sum D_{Ri}\right)$$

Here ΣD_A is the sum of all advective processes and ΣD_R is the sum of all reaction processes. Although this model can be used to simulate the release of PCBs from a sunken vessel, without accounting for the potential resistances associated with media transfers from water, the water concentration may be under-estimated while other phase concentrations (e.g., sediment, DOC, and air) may be over-estimated. Because of this and USEPA review comments on PRAM Version 1.3, the Level II modeling approach was not considered to be sufficiently refined. Therefore, PRAM Version 1.4c was developed based on the Level III fugacity modeling approach (PRAM Version 1.3 used a Level II fugacity modeling approach, e.g., see Goodrich et al., 2003).

2.5.1.3 Model III Fugacity Model

Unlike the Level II model, the Level III model does not assume equilibrium (a common fugacity) between the phases or compartments within the system. Transfer resistances control the exchange between the compartments within the system. In addition to advection and reactive processes, the Level III model considers diffusion/dispersive processes. This modeling approach is considered to be more refined or "accurate" for environmental modeling as true equilibrium among phases (compartments) is considered rare within the real world and diffusive resistance can affect intermedia (inter-"compartmental") transfers at the respective boundaries.

Intermedia mass transfers can occur through both advective processes and diffusive processes within the Level III modeling scheme. PCB transfers can be expressed as $D_{ij}f$ where the diffusivity D_{ij} term includes those processes affecting diffusion, including resistance and f is the compartmental fugacity (see Mackay et al., 1985; Mackay and Paterson, 1991). The nomenclature for the D (transport) term within the Level III, as used here, is represented by D_A and D_R, which are advective and reactive transport terms, respectively, while D_{ij} refers to *total* (advective and diffusive) transport terms between media (phases and/or compartments) within the system. By invoking system steady-state conditions, a mass balance using the fugacity approach can be illustrated for each system compartment where inputs are balanced by outputs. This approach results in no net gain or loss of the chemical within the system, despite varied exchanges or non-common fugacities or "escape tendencies" between compartments (common fugacities are assumed to occur within individual compartments). This approach is represented by the following equation for delineating the transport mechanism in terms of mass emission, N [mol/day], across the entire system (see Mackay, 1985; Mackay and Paterson, 1991):

$$(20)\quad N - f_i\left(\sum_j D_{ij} + D_{Ai} + D_{Ri}\right) + \sum_j\left(D_{ji} f_j\right) = 0$$

where:
i = compartment or phase i
f_i = the fugacity of phase / compartment i
f_j = the fugacity of phase / compartment j
D_{ji} = the transport coefficient(s) from compartment j into compartment i

The foregoing equation is easily rearranged to solve for the compartmental fugacity (f_i):

$$(21)\quad f_i = \frac{N + \sum_j\left(D_{ji} f_j\right)}{\sum_j\left(D_{ij} + D_{Ai} + D_{Ri}\right)}$$

Compartmental concentrations can then be calculated using the compartmental fugacity and Z value for the media just as previously described for the Level II model. The transport terms, which include diffusive transport, for the PRAM system are shown in Figure 6 coupled to the exchanges they represent.

As discussed in the beginning of this section, the Level III model is the most represented in the scientific literature in the context of environmental modeling and is the level of modeling used within the PRAM Version 1.4c.

2.5.1.4 Model IV Fugacity Model

A Level IV fugacity model is a true dynamic model in that both space and time are modeled dynamically. The model system is not considered to be at equilibrium. Nor is it considered to be at steady-state. The exchanges are not assumed to balance because fluxes to and from compartments are not balanced. This is reflected in the fugacity equation where:

$$N - f_i\left(\sum_j\left(D_{ij} + D_{Ai} + D_{Ri}\right)\right) + \sum_j\left(D_{ji} f_j\right) \neq 0$$

(22) and as such :

$$ViZi\frac{\partial f}{\partial t} = N^t - f_i\left(\sum_j\left(D_{ij} + D_{Ai} + D_{Ri}\right)\right) + \sum_j\left(D_{ji} f_j\right)$$

where t = time

Solutions for the fugacity terms within Level IV cannot be made through simple algebra as for model Levels I, II, and III. The Level IV fugacity model requires significantly more data inputs than any of the preceding structures to describe fluxes within the system. While empiric equilibrium constants such as organic carbon partitioning coefficients (K_{oc}s) are functional in lower levels of fugacity modeling, time specific rates of for such processes are required for this model (e.g., rate of absorption and desorption). The Level IV model is mathematically and data intensive but does not appear to significantly differ from Level III in the model's ability to account for pollutant inventories (Hertwich, 2001). Further, in a direct comparison between a steady-state Level III and non-steady-state Level IV fugacity modeling approach, Hertwich (2001) concluded the important properties such as a dose, persistence and spatial distribution can be equally derived from the Level III as with the Level IV model. Based on such information, the additional data requirements, and the desire to, as stated by many (e.g., Trapp and Matthies, 1996; Mackay et al., 1995; and others) minimize model development complexity to assure confidence in data inputs and future validation, the Level IV model was not considered the most appropriate for the PRAM.

2.5.2 PRAM Level III Fugacity Model and Algorithms

In the PRAM Level III fugacity construct, PCB exchange occurs between five compartments (see Figure 6):

- An air body bounded vertically by the atmosphere to water surface and laterally by a user input value[17]

[17] This lateral input value defines the lateral "zone of influence or ZOI" for the artificial reef created by the sunken vessel.

- A water body above the pycnocline bounded by the water surface and laterally by a user input value
- A water compartment within the vessel interior
- A water compartment outside of the vessel bounded by a respective lateral user input value and vertically by the pycnocline,[18]
- A sediment bed bounded in depth and laterally by a user input value

These five compartments within the PRAM are treated as "bulk" compartments within which there are sub-compartments of particles, water, and dissolved organic carbon, as appropriate (see Section 2.1). These compartments are treated as bulk phases (e.g., see Mackay and Paterson, 1991), and as such, the fugacity capacity (Z value) of each phase is weighted by the fractional portion of the sub-compartments. For example, compartment 2 (upper water column) consists of water, suspended particles, and dissolved organic carbon. The fugacity capacity for the upper water column as a bulk phase is represented by the following equation:

$$(23)\quad Z_2 = \phi Z_{\text{water}} + \phi Z_{\text{suspended - sediment}} + \phi Z_{\text{dissolved organic carbon}}$$

Where ϕ is the volume fraction of the specific media within compartment 2 (the upper water column) and the Z is the respective fugacity capacity for the media listed.

A nomenclature using the compartment numbers can be used to simplify the description of this weighting process where the first subscript for the Z value represents the compartment and the second represents the media within that compartment[19] (A = air, W = water, SS = suspended particles, AE = aerosols, SD = sediment, and DOC = dissolved organic carbon).

Air Compartment

$$(24)\quad Z_1 = \phi_{1A} Z_A + \phi_{1AE} Z_{AE}$$

Upper Water Column Compartment

$$(25)\quad Z_2 = \phi_{2W} Z_W + \phi_{2SS} Z_{SS} + \phi_{2DC} Z_{DOC}$$

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[18] Per the November 17/18, 2004 TWG meeting, EPA recommended pycnocline to be used as the vertical boundary.

[19] Not all media listed are present in all compartments, e.g., no air is present in the sediment bed, etc.

Lower Water Column Compartment

(26) $Z_3 = \phi_{3W} Z_W + \phi_{3SS} Z_{SS} + \phi_{3DC} Z_{DOC}$

Sediment Bed Compartment

(27) $Z_4 = \phi_{4SD} Z_{SD} + \phi_{4W} Z_W + \phi_{4DOC} Z_{DOC}$

Sunken Vessel Interior Compartment

(28) $Z_5 = \phi_{5W} Z_W + \phi_{5SS} Z_{SS} + \phi_{5DC} Z_{DOC}$

Transfers of PCBs can occur between these compartments and through these compartments to the outside of the system (Level III fugacity model is an open system). Additionally, the sub-compartments can also carry PCBs into adjacent compartments via advection. The mass transfers or exchanges of PCBs considered relevant for the PRAM are presented in Table 4 (Transfer Coefficients) and illustrated in Figure 6.

2.5.2.1 Non-Diffusive Transport Within the PRAM

The compartmental exchanges/transfers or "intermedia transfer parameters" are defined as transfer coefficients or D terms as described above. *Non-diffusive* transports (advective and reactive [biodegradation]) are described below for the PRAM compartments:

Compartment 1 – Air compartment
Non-diffusive transport within this compartment is enabled by precipitation, specifically:

Rain;
(29) $D_{QW} = A_{12} \times U_Q \times Z_W$

Wet particle deposition;
(30) $D_{DW} = A_{12} \times U_Q \times \phi_{1AE} Z_{AE}$

Dry particle deposition;
(31) $D_{PW} = A_{12} \times U_P \times \phi_{1AE} Z_{AE}$

Physical advection out of the compartment;

(32) $D_{A1} = G_A \times Z_1$

where:
A_{12} = the surface area of the water – air interface (m^2)
U_Q = the rain rate (m^3 rain/m^2 area –day)
U_P = dry deposition velocity (m/day)
G_A = air flow through the air compartment (m^3/day)
= [air current x cross-sectional area]
ϕ = the volume fraction of the specific media within compartment 1 and Z values as previously defined

Compartment 2 – Upper water column compartment

Physical advection out of the compartment;

(33) $D_{A2} = G_{W2} \times Z_2$

Biodegradation;

(34) $D_{R2} = K_W \times V_{2W} \times \phi_{2w} Z_W$

where:
G_{W2} = water flow through the upper water column compartment (m^3/day)
= [current x cross-sectional area]
K_w = rate of biodegradation of PCB in water (1/day)
V_{2W} = the volume of pure water in compartment 2 (m^3)
ϕ = the volume fraction of the specific media within compartment 2 and Z values as previously defined

Compartment 3 – Lower water column compartment

Physical advection out of the compartment;

(35) $D_{A3} = G_{W3} \times Z_3$

Biodegradation;

(36) $D_{R3} = K_W \times V_{3W} \times \phi_{3w} Z_W$

where:
G_{W3} = water flow through the lower water column compartment (m^3/day)
= [current x cross-sectional area]
K_w = rate of biodegradation of PCB in water (1/day)
V_{3W} = the volume of pure water in compartment 3 (m^3)
ϕ = the volume fraction of the specific media within compartment 3 and Z values as previously defined

Compartment 4 – Sediment bed compartment

Particulate deposition;

(37) $D_{DX} = A_{34} \times U_{DX} \times \phi_{3ss} Z_{SS}$

Particulate resuspension;

(38) $D_{RX} = A_{34} \times U_{RX} \times \phi_{4SD} Z_{SD}$

Sediment burial;

(39) $D_B = A_4 \times U_B \times \phi_{4SD} Z_{SD}$

Biodegradation;

(40) $D_{R4} = K_W \times V_{4W} \times \phi_{4sd} Z_W$

where:
A_{34} = surface area for sediment bed – water column interface (m^2)
U_{DX} = suspended solid deposition velocity (m/day)
U_{RX} = sediment re-suspension solid velocity (m/day)
A_4 = surface area for sediment bed (m^2)
U_B = sediment burial velocity (m/day)
K_w = rate of biodegradation of PCB in water (1/day)
V_{4W} = the volume of pure water in sediment bed - compartment 4 (m^3)
ϕ = the volume fraction of the specific media within compartment 4 and Z values as previously defined

Compartment 5 – Sunken vessel interior compartment

Physical advection out of the compartment;

(41) $D_{A5} = G_{W5} \times Z_5$

Biodegradation;

(42) $D_{R5} = K_W \times V_{5W} \times \phi_{5W} Z_W$

where:
G_{W5} = total flux from the interior vessel compartment (m^3/day)
= [current x cross-sectional area]
K_w = rate of biodegradation of PCB in water (1/day)
V_{5W} = the volume of pure water in compartment 5 (m^3)
ϕ = the volume fraction of the specific media within compartment 5 and Z values as previously defined

These non-diffusive transport coefficients are combined with the diffusive transport coefficients defined below to quantify total transport between compartments and ultimately the compartmental fugacities required to calculate each phase PCB concentration.

2.5.2.2 Diffusive Transport Within the PRAM

Three diffusive exchanges are considered within the PRAM:

- PCB exchange between the upper water column (compartment 2) and air (compartment 1) across the water–air boundary layer,
- PCB exchange between the lower water column (compartment 3) and the upper water column (compartment 2) across the pycnocline, and
- PCB exchange between the lower water column (compartment 3) and the pore water within the sediment bed (compartment 4) across the sediment bed–surface water boundary layer.

These exchanges are bi-directional but the net flux of PCBs is based on the concentration gradient between the exchanging compartments. Exchange of PCBs between compartments involves both molecular diffusion and turbulent diffusion (dispersion). As described previously, the forcing process for diffusive flux across a boundary layer is the concentration gradient, which can be described as:

(6) $$N_{diff} = A\left[m^2\right]\times\left(\frac{D\left[\frac{m^2}{day}\right]}{\Delta[m]}\times\left(C_2\left[\frac{mol}{m^3}\right]-C_1\left[\frac{mol}{m^3}\right]\right)\right)$$

where:
N = net substance diffusive flux due to diffusion and turbulence (mol/day)
A = the surface area
D = the diffusion coefficient
$C_2 - C_1$ = the concentration gradient
Δ = the "thickness" of the boundary or diffusion gradient

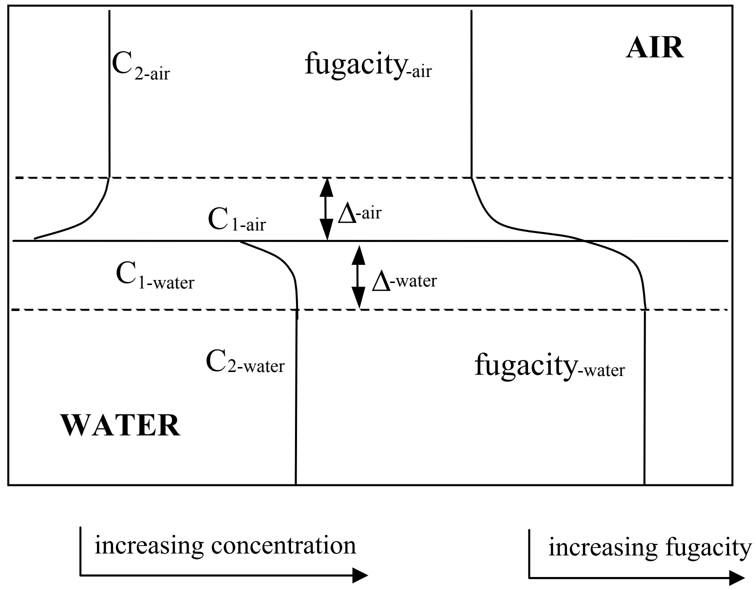
Salient for the modeling scheme here is a mass transfer coefficient (MTC), which is dissected from the above equation as D/Δ across a concentration gradient, and working at a level of flux per unit area where:

(43) $$N\left[\frac{mol}{m^2 \cdot day}\right] = \frac{D}{\Delta}\left(C_2 - C_1\right) = U\left(C_2 - C_1\right)$$

where:
U = MTC = D/Δ

2.5.2.3 Surface Water and Air Diffusive Boundary

An illustration of the boundary condition between upper water column (compartment 2) and air (compartment 1) is presented below (adapted from UCD and LLNL, 1994):



The air concentration above the laminar layer (represented by the dotted line above the water surface) is assumed to be well-mixed and homogenous in concentration. Similarly, the water concentration below the laminar layer just below the water surface is represented by a single concentration. These two well-mixed compartmental concentrations are related to the fugacity capacities of the compartments where diffusive processes are considered such that:

$$(44)\quad N\left[\frac{mol}{m^2\cdot day}\right]=Y_{aw}\left[\frac{mol}{m^2\cdot Pa\cdot day}\right]\left(f_{air}[Pa]-f_{water}[Pa]\right)$$

where Y_{aw} is the overall fugacity mass transfer coefficient per day

Considering that diffusive flux will occur in two directions at a boundary layer using the air–water boundary, the flux to the airside of the boundary from the water and from the air to waterside of the boundary must balance or:

$$(45)\quad N=U_a\left(C_{2-air}-C_{1-air}\right)$$

and

$$(46)\quad N=U_w\left(C_{2-water}-C_{1-water}\right)$$

where $C_{1\text{-}air}$, $C_{2\text{-}air}$, $C_{1\text{-}water}$, and $C_{2\text{-}water}$ are concentrations near the boundary layer as shown above.

Noting that at the surface the partitioning between water and air can be expressed in terms of their Z values:

$$(47)\quad \frac{C_{1-air}}{C_{1-water}} = \frac{Z_A}{Z_W}$$

and also noting that C = fZ_1 within each compartment, the foregoing equations can be manipulated to replace the concentration terms with Z values (see UCD and LLNL, 1994 for the specific algebraic manipulations):

$$(48)\quad Y_{aw} = \left(\frac{1}{Z_A \times U_a} + \frac{1}{Z_W \times U_w} \right)^{-1}$$

This overall fugacity mass transfer coefficient is related to the airside and waterside mass transfer coefficients where:

airside;

$$(49)\quad Y_{aw}^{a} = Z_A U_a = Z_A \left(\frac{D_a}{\Delta_a} \right)$$

waterside;

$$(50)\quad Y_{aw}^{w} = Z_W U_w = Z_W \left(\frac{D_w}{\Delta_w} \right)$$

The CalTOX model (UCD and LLNL, 1994) as well as the CemoS Model (Baumgarten et al., 1996) use an empiric method to estimate D/Δ based on the laboratory results of Southworth (1979). However, the data used by Southworth (1979) was specific to a large freshwater river (see Trapp and Harland, 1995). The approach suggested for open ocean is that of Liss and Slater (1974), which is specific to the air–ocean interface. Liss and Slater (1974) determined that the average transfer velocity (the combination of diffusion velocity and turbulence) for water across the seawater – air interface was 30 m/hour.

Two other methods in addition to the Southworth and Liss and Slater methods were compared to field observations by Trapp and Harlan (1995), that of Mackay and Yeun (1983) which was developed for lake environments, and the method presented as the Langbein–Durum method (Tapp and Harland, 1995) for a river backwater situation. For prospective, in the seminal papers of Mackay (Mackay et al., 1985; Mackay and Paterson, 1991) a mass transport coefficient (U) of 3 m/hour (72 m/day) for the airside U coefficient and 0.03 m/hour (0.72 m/day) for the waterside U coefficient were used in modeling hexa-CB. According to Mackay and Paterson (1991), these values were selected based on best professional judgment without any further justification.

Given that the PRAM is attempting to model all ten homolog series with significantly different diffusion coefficients (D), the use of a single U for all seems too simplistic while the development of ten values based on best professional judgment seems too much of a task. It seems appropriate that the methods that could account for the variable chemical diffusivities of the PCBs as well as potentially, wind speed and water current, be considered as part of the PRAM development.

Trapp and Harland (1995) evaluated the aforementioned four estimation methods for a large river and a ship channel. Although neither situation is similar to the open ocean application anticipated for the PRAM, the relative performances of the models are useful here. The Liss and Slater method over-estimated the observed transport velocities for both situations (Trapp and Hartland, 1995). Both the Southworth and Langbein–Durum methods significantly under-estimated the velocities for the ship channel scenario but were accurate predictors of the river scenario. The Mackay and Yeun method significantly under-estimated the transport velocity for the river scenario and significantly over-estimated the velocity for the ship channel (Trapp and Hartland, 1995). The lone method for oceans appears to produce non-conservative results based on the limited attempt by Trapp and Hartland (1995) to validate the model. Although, as pointed out by Trapp and Hartland (1995), “It is unlikely that one universal empirical model is applicable to all cases and consequently no exact simulation can be expected,” it is believed that a conservative algorithm can be deduced. The Southworth method was consistently conservative or accurate in the validation scenarios reported by Trapp and Hartland, although overly conservative under certain situations of very low current speeds (Trapp and Hartland, 1995).

Based on the apparent conservatism associated with the Southworth method and the precedence for its use within CemoS and CalTOX, the method has been adopted for use within the PRAM. One perhaps significant uncertainty for the application of this approach is that the method was derived with chemicals with Henry’s Law Constants between 1 and 100 Pa and some of the more chlorinated PCB homolog series have much higher Henry’s Law constants. The impact of this is unclear at this time.

Using the Southworth method, as described by UCD and LLNL (1994), the mass transfer coefficient on the waterside (U_w) is calculated as follows:

$$\text{(51) where current}\left[\frac{m}{\sec}\right] < 0.04 \times \text{wind}\left[\frac{m}{\sec}\right]^{0.67}; U_w = 0.24\left[\frac{m}{day}\right]$$

$$\text{where (51) is not true and where wind}\left[\frac{m}{\sec}\right] < 1.9\left[\frac{m}{\sec}\right] \text{(3.7 knots);}$$

$$\text{(52)} \quad U_w\left[\frac{m}{day}\right] = 5.64\left(\frac{\text{current}\left[{}^{m}\!/_{\sec}\right]^{0.969}}{\text{water depth}\,[m]^{0.673}}\right) \times \sqrt{\frac{32}{MW_{PCB-series}}}$$

$$\text{where (51) is not true and where wind}\left[\frac{m}{\sec}\right] > 1.9\left[\frac{m}{\sec}\right]$$

$$\text{(53)} \quad U_w\left[\frac{m}{day}\right] = 5.64\left(\frac{\text{current}\left[{}^{m}\!/_{\sec}\right]^{0.969}}{\text{water depth}\,[m]^{0.673}}\right) \times \sqrt{\frac{32}{MW_{PCB-series}}} \times e^{0.526(wind-1.9)}$$

Water depth in the context of the PRAM is the depth to the pycnocline, which represents a second boundary layer. $MW_{PCB\text{-}series}$ is the molecular weight for a particular homolog series.

For the airside mass transfer coefficient (U_a) according to Southworth (1979, as cited in UCD and LLNL, 1994):

$$\text{(54) where current}\left[\frac{m}{\sec}\right] + \text{wind}\left[\frac{m}{\sec}\right] < 0.5\left[\frac{m}{\sec}\right] \text{(0.97 knots);}$$

$$\text{(55)} \quad U_a\left[\frac{m}{day}\right] = 140\sqrt{\frac{18}{MW_{PCB-series}}}$$

$$\text{where current}\left[\frac{m}{\sec}\right] + \text{wind}\left[\frac{m}{\sec}\right] > 0.5\left[\frac{m}{\sec}\right];$$

$$\text{(56)} \quad U_a\left[\frac{m}{day}\right] = 273\left(\text{wind}\left[\frac{m}{\sec}\right] + \text{current}\left[\frac{m}{\sec}\right]\right)\sqrt{\frac{18}{MW_{PCB-series}}}$$

Diffusive transport across the air–surface water boundary in terms of the fugacity D value (D_v, in mol/Pa-day) requires a surface area for the interface (m^2) and is calculated as, using the nomenclature within the PRAM for compartmental exchanges:

$$(57) \quad D_v = \frac{1}{\left[\frac{1}{(U_{12} Z_A A_{12})} + \frac{1}{(U_{21} Z_W A_{12})} \right]}$$

where U_{12} is the airside mass transfer coefficient for the air-to-surface water boundary and U_{21} is the waterside mass transfer coefficient for the surface water-to-air boundary.

2.5.2.4 Lower Water Column and Upper Water Column Diffusive Boundary

No empiric method is available for estimating the mass transfer coefficients for the diffusive exchange of PCBs between the upper water column and lower water column across the pycnocline (PRAM compartments 2 and 3, respectively). There is, however, enough evidence for the transport of nutrients across the pycnocline that an effective diffusive value of 0.1 cm^2/sec (0.864 m^2/day) has been suggested. Additionally the thickness of the pycnocline is assumed to equal 1 meter and as such, the diffusion path for each side of this boundary is 0.5 m. The foregoing assumptions simplify the overall fugacity mass transport coefficient and D values to:

$$(58) \quad D_w = \frac{1}{\left[\frac{1}{\left(\frac{0.864 m^2}{d} (0.5\, m)^{-1} \right) (Z_W A_{23})} + \frac{1}{\left(\frac{0.864 m^2}{d} (0.5\, m)^{-1} \right) (Z_W A_{23})} \right]}$$

2.5.2.5 Lower Water Column and Sediment Bed Diffusive Boundary

The last boundary considered within the PRAM is that between the lower water column and the sediment bed (PRAM compartments 3 and 4, respectively). Diffusion will occur within the water phase within the sediment bed, which is affected by the void space within the sediment bed. Mackay and Paterson (1991) do not take into account any impact due to the presence of solids along the diffusion pathway. The CalTOX model does include a correction of the presence of particles within the sediment bed based on the work of

Millington and Quirk (1961) that would reduce the efficiency of the diffusion process along a path where the effective diffusion (D_{eff}) is defined as:

$$(59) \quad D_{eff} = \left(\omega^{10/3} / \phi^2 \right) D_w$$

where:

ω = the void fraction of the media occupied by the liquid[20]

ϕ = the total void fraction within the media

In sediment, the entire void fraction is occupied by water such that the equation within the PRAM is stated as:

$$(60) \quad D_S = \left(\phi^{10/3} / \phi^2 \right) D_w = \phi^{\frac{4}{3}} DW$$

where D_S is the effective diffusion within the sediment pore water.

The waterside and sediment-side mass transfer coefficients are then expressed as:

waterside;

$$(61) \quad Y_{ws}^{w} = Z_W U_{34} = Z_W \left(\frac{D_W}{\Delta_{34}} \right)$$

sediment – side;

$$(62) \quad Y_{ws}^{w} = Z_W U_{34} = Z_W \left(\frac{D_W}{\Delta_{34}} \right)$$

The interface between sediment and surface water can be diffuse where the thickness of the waterside boundary layer is difficult to define. The CalTOX model (UCD and LLNL, 1994) used a static value of 0.020 m, based on a study of radon transfers in the Hudson River (Hammond et al., 1975, as cited in UCD and LLNL, 1994). The use of a static value can

[20] The original equation is designed to account for the presence of additional liquids and air within the void space.

constrain the analysis and as the value is based on a river study where sediment bed stability and currents above the bed may be quite different than that of an artificial reef environment, the CalTOX default value may not be applicable. Mackay et al. (1985) and Mackay and Paterson (1991) did not explicitly set the boundary thickness and used a transport coefficient (equivalent to U_{34} here) of 0.01 m/hour. As with the CalTOX approach, this is a static value and while believed to be functional, it is less desirable as it will not account for the differences in diffusion coefficients for the ten PCB homolog series evaluated by the PRAM. Additionally, comments from the TWG suggest that the boundary thickness along the seafloor in the area of the ex-ORISKANY Memorial Reef would be just a few centimeters. Until more relevant data become available, the 0.020 m (2 cm) as used by the CalTOX model is assumed to be functional for the PRAM.

As for the sediment-side boundary layer thickness, Mackay and Paterson (1991) used half of the depth of the defined active sediment bed (i.e., the bioturburation zone, see Bosworth and Thibodeaux, 1990), which is a common practice (e.g., see USEPA, 1982; Trapp and Matthies, 1996).

The CalTOX model approached this issue differently where a functional relationship between outputs from the Jury et al. (1983) modeling approach for soils were regressed against a range of effective diffusion coefficients for chemicals with a wide range of K_{oc}s and Henry's constants (UCD and LLNL, 1994). The following relationship was established and is used by CalTOX to estimate the sediment-side boundary thickness:

$$(63) \quad \Delta_{43}[m] = 318 \quad D_S^{0.683}$$

There is some uncertainty associated with this approach because model results are used as inputs to a subsequent modeling scheme and the applicability of predicted soil results for sediment may not be valid. The appropriateness of this approach within the PRAM is unclear, as it would suggest the diffusion path length varies for each PCB homolog series. Because of this, and given the uncertainties associated with the use of a soil-based model result, the CalTOX model was rejected for this purpose. The approach used by Mackay et al. (1985) and many others, where the diffusion path length or boundary thickness for sediment is set as half of the active sediment layer, is used within the PRAM.

Diffusive transport across the surface water – sediment bed boundary in terms of the fugacity D value (D_v, in mol/Pa-day) requires a surface area for the interface (m^2) and is calculated as follows, using the nomenclature with PRAM for compartmental exchanges:

$$(64)\quad D_Y = \frac{1}{\left[\frac{1}{(U_{34} Z_W A_{34})} + \frac{1}{(U_{43} Z_W A_{43})} \right]}$$

where U_{34} is the waterside mass transfer coefficient for the surface water to sediment bed boundary and U_{43} is the sediment-side mass transfer coefficient for the sediment bed to surface water.

2.5.2.6 Compartmental Fugacities and Media PCB Concentrations

By invoking steady-state conditions, a mass balance using the fugacity Level III approach can be illustrated (see also Figure 7) for each compartment where inputs are balanced by outputs as follows (see Mackay, 1985; Mackay and Paterson, 1991):

$$(65)\quad N - f_i \sum_j (D_{ij} + D_{Ai} + D_{Ri}) + \sum_j (D_{ji} f_j) = 0$$

Algebraic rearrangement results in a solution for the compartmental fugacity:

$$(66)\quad f_i = \frac{N + \sum_j (D_{ji} f_j)}{\sum_j (D_{ij} + D_{Ai} + D_{Ri})}$$

Where there is no direct emission into the compartment[21] except for those transfers from adjacent compartments, the foregoing simplifies to:

$$(67)\quad f_i = \frac{\sum_j (D_{ji} f_j)}{\sum_j (D_{ij} + D_{Ai} + D_{Ri})}$$

Thus, using Table 4, the individual fugacity (*f*) for each compartment (as a bulk media) can be calculated:

$$(68)\quad f_5[\text{Pa}] = \frac{N_5[\text{mol/hr}]}{D_{A_5}[\text{mol/Pa}-\text{hr}]}$$

Advection (DA) is considered to be the sole driving force for transporting the released PCBs from the interior of the vessel bulk water compartment (compartment 5) into the surrounding water column. It is notable that the advection term is for bulk water leaving the compartment that includes PCBs attached to suspended solids and dissolved organic carbon.

The lower water column (compartment 3, the bulk water below the pycnocline) receives the discharge of PCBs from the vessel interior:

$$(69)\quad f_3 = \frac{D_{53}f_5 + D_{23}f_2 + D_{43}f_4}{D_{32} + D_{34} + D_{A_3} + D_{R_3}}$$

The release of PCBs from the interior of the vessel into the lower water column is an advection term for a physical/mass input into the lower water column. This water compartment loses and gains PCBs from the upper water column (water above the pycnocline) and the sediment bed via diffusion and dispersion and losses PCBs advectively and through degradation.

The lower water compartment has functional[22] boundaries with the sediment bed and the upper water column such that diffusive transport into these compartments is a salient issue. The fugacity of the sediment bed compartment, in recognition of its connection with the lower column, is as follows:

$$(70)\quad f_4 = \frac{D_{34}f_3}{D_{43} + D_{R_4} + D_{Bs}}$$

The bulk sediment bed (compartment 4) gains and loses PCBs via dispersive processes from the lower water column and loses PCBs through degradation and sediment burial.

[21] Compartment 5 (the vessel interior) is the only compartment within the PRAM that receives direct emissions of PCBs.

[22] No diffusive boundary is considered to be present between the vessel interior water compartment and the lower water column compartment.

PCBs, based on this model, are transported into the upper water column (compartment 2) from the lower water column via dispersive process across the pycnocline (2-way process) and across the boundary with bulk air (compartment 1) such that the fugacity of the upper bulk water column is algebraically described as:

$$(71)\quad f_2 = \frac{D_{32} f_3 + D_{12} f_1}{D_{21} + D_{23} + D_{A_2} + D_{R_2}}$$

For bulk air (compartment 1) the compartmental fugacity is:

$$(72)\quad f_1 = \frac{D_{21} f_2}{D_{12} + DA_1}$$

No reactive processes are assumed to occur in the atmosphere, which is considered to be a conservative assumption as it conserves PCBs. While the forgoing algebraic solutions are correct they are circular solutions such that extensive substitution is required to mathematically solve the equations.[23] The substitutions are provided in Appendix D and the solutions are as follows:

$$(73)\quad f_3 = \frac{D_{53} f_5}{DT_3 - \dfrac{D_{23} D_{32} DT_1}{DT_1 DT_2 - D_{12} D_{21}} - \dfrac{D_{34} D_{43}}{DT_4}}$$

$$(74)\quad f_4 = \frac{D_{34} f_3}{DT_4}$$

$$(75)\quad f_2 = \frac{D_{32} f_3}{DT_2 - \dfrac{D_{12} D_{21}}{DT_1}}$$

$$(76)\quad f_1 = \frac{D_{21} \times \dfrac{D_{32} f_3}{DT_2 - \dfrac{D_{12} D_{21}}{DT_1}}}{DT_1}$$

Given the fugacity for each compartmental phase (air, upper water column, lower water column, sediment, and vessel interior water), the bulk concentrations and intracompartmental media concentrations can be calculated. Bulk compartmental concentrations are calculated per equation 17, where concentration (mols/m^3) is defined by: $C = Zf$. Thus, in the context of the bulk concentrations for each compartment and each PCB homolog series:

$$\text{(77)} \quad \mathrm{PCB}_{1-\mathrm{air}}\left[{}^{mg}\!/\!{}_{L}\right] = Z_1 \times f_1 \times \text{PCB Molecular weight}\left[\frac{g}{mol}\right]$$

$$\text{(78)} \quad \mathrm{PCB}_{2-\mathrm{upper-water}}\left[{}^{mg}\!/\!{}_{L}\right] = Z_2 \times f_2 \times \text{PCB Molecular weight}\left[\frac{g}{mol}\right]$$

$$\text{(79)} \quad \mathrm{PCB}_{3-l\mathrm{ower-water}}\left[{}^{mg}\!/\!{}_{L}\right] = Z_3 \times f_3 \times \text{PCB Molecular weight}\left[\frac{g}{mol}\right]$$

$$\text{(80)} \quad \mathrm{PCB}_{4-\mathrm{sedimentbed}}\left[{}^{mg}\!/\!{}_{L}\right] = Z_4 \times f_4 \times \text{PCB Molecular weight}\left[\frac{g}{mol}\right]$$

$$\text{(81)} \quad \mathrm{PCB}_{5-\mathrm{vessel\text{-}interior}}\left[{}^{mg}\!/\!{}_{L}\right] = Z_5 \times f_5 \times \text{PCB Molecular weight}\left[\frac{g}{mol}\right]$$

The specific media concentrations within each compartment are calculated using the compartmental fugacity, the media fugacity capacities, and densities (ρ in g/mol) of the media where:

In compartment 1 (the air compartment)

$$\text{(82)} \quad \mathrm{PCB}_{air}\left[{}^{g}\!/\!{}_{m^3}\right] = Z_A \times f_1 \times \text{PCB Molecular weight}\left[\frac{g}{mol}\right]$$

$$\text{(83)} \quad \mathrm{PCB}_{aerosols}\left[{}^{mg}\!/\!{}_{kg}\right] = \left(Z_{AE} f_1 \times \text{PCB Molecular weight}\left[\frac{g}{mol}\right]\right) \Big/ \rho_{aerosols}\left[\frac{g}{cm^3}\right]$$

[23] Matrix solutions are possible within the code of the program given the absolute values for the input parameters using Gaussian elimination matrix techniques, what is presented here and in Appendix D is a pure

In compartment 2 (the upper water column)

$$(84)\quad \text{PCB}_{Water}\left[{}^{mg}\!/\!{}_{L}\right] = Z_W \times f_2 \times \text{PCB Molecular weight}\left[\frac{g}{mol}\right]$$

$$(85)\quad \text{PCB}_{\text{Suspended Solids}}\left[{}^{mg}\!/\!{}_{kg}\right] = \left(Z_{SS} \times f_2 \times \text{PCB Molecular weight}\left[\frac{g}{mol}\right]\right) \Big/ \rho_{\text{SS}}\left[\frac{g}{cm^3}\right]$$

$$(86)\quad \text{PCB}_{\text{Dissolve Organic Carbon}}\left[{}^{mg}\!/\!{}_{kg}\right] = \left(Z_{DC} \times f_2 \times \text{PCB Molecular weight}\left[\frac{g}{mol}\right]\right) \Big/ \rho_{\text{DC}}\left[\frac{g}{cm^3}\right]$$

The formats for the media concentrations in compartment 3 (the lower water column) are the same as those for the upper water column (compartment 2) except that the fugacity used is specific to compartment 3 (f_3). For compartment 4 (the sediment bed), the media concentrations are calculated as:

$$(87)\quad \text{PCB}_{\text{Sediment}}\left[{}^{mg}\!/\!{}_{kg}\right] = \left(Z_{\text{SD}} \times f_4 \times \text{PCB Molecular weight}\left[\frac{g}{mol}\right]\right) \Big/ \rho_{\text{sediment}}\left[\frac{g}{cm^3}\right]$$

$$(88)\quad \text{PCB}_{Pore-water}\left[{}^{mg}\!/\!{}_{L}\right] = Z_W \times f_4 \times \text{PCB Molecular weight}\left[\frac{g}{mol}\right]$$

$$(89)\quad \text{PCB}_{\text{DOC in pore water}}\left[{}^{mg}\!/\!{}_{kg}\right] = \left(Z_{DC} \times f_4 \times \text{PCB Molecular weight}\left[\frac{g}{mol}\right]\right) \Big/ \rho_{\text{DC}}\left[\frac{g}{cm^3}\right]$$

algebraic solution.

and within the sunken vessel (compartment 5)

$$(90)\quad PCB_{Water}\left[{}^{mg}\!/_{L}\right] = Z_W \times f_5 \times \text{PCB Molecular weight}\left[\frac{g}{mol}\right]$$

$$(91)\quad PCB_{\text{Suspended Solids}}\left[{}^{mg}\!/_{kg}\right] = \left(Z_{SS} \times f_5 \times \text{PCB Molecular weight}\left[\frac{g}{mol}\right]\right) \Big/ \rho_{SS}\left[\frac{g}{cm^3}\right]$$

$$(92)\quad PCB_{\text{Dissolve Organic Carbon}}\left[{}^{mg}\!/_{kg}\right] = \left(Z_{DC} \times f_5 \times \text{PCB Molecular weight}\left[\frac{g}{mol}\right]\right) \Big/ \rho_{DC}\left[\frac{g}{cm^3}\right]$$

2.6 THE PRAM FOOD WEB AND TROPHIC TRANSFERS OF PCBS

The PRAM models the transfer of PCBs from abiotic media into biota mechanistically. The structure of the food web within which the released PCBs are transferred is treated as a closed system. That is, all of the components (organisms) are assumed to be resident within the model construct, and do not spend any time or obtain any food outside the influence of the sunken vessel. For sessile organisms and less mobile organisms associated with the reef structure and nearby sediment bed, this assumption is probably accurate. However, for mobile organisms such as fish, this is a highly conservative approach, as many fish are known to move from reef to reef and undergo seasonal and/or life-stage migrations. This is especially true for pelagic organisms, a major community modeled by PRAM where the vast majority of such species undergo large oceanic movements over their lifetime.

2.6.1 Food Web Communities Considered Within the PRAM

Three distinct biological communities are modeled within PRAM: a reef community, a benthic community, and a pelagic community. This approach was taken based on differences in habitat and dietary exposure anticipated among different groups of marine organisms that would likely be found in the vicinity of an artificial reef, as well as information on the fishing techniques used by anglers and the apparent distribution of sport fish "types" taken from artificial reefs such as the ex-VERMILION.[24]

[24] In performing the human health risk assessment for the ex-VERMILION artificial reef off the coast of South Carolina, the Navy, assisted by the Marine Resources Division/Department of Natural Resources (SCDNR),

One study, focusing on natural hard bottom habitats in the general vicinity of the proposed ex-ORISKANY Memorial Reef site (Thompson et al., 1999), and other studies broader in area (e.g., Bortone et al., 1997) indicate substantial variability in biotic community composition with both sea depth and "shape" of submerged structures. Considering the available relevant literature, and the unusual size and shape of the ex-ORISKANY relative to other structures that have been studied, it is difficult to accurately predict community composition and/or structure in detail. The habitats provided by the vessel will almost certainly be exploited by a wide range of transient and (at least effectively) resident fishes. Thus, the communities associated with the sunken vessel are described and modeled in general, as described in the following paragraphs.

Each of the three communities within the PRAM is subdivided into "trophic" levels. The term "trophic" relates to nutrition (source of energy) and trophic "level" refers to a position relative to original source of energy input into the food web (i.e., feeding relationships among plants and animals in a certain area). Trophic Level I refers to the primary producers (i.e., plants such as algae), which capture energy from non-living material and an energy source, particularly sunlight. Those organisms that feed directly on the primary producers would be classified as Trophic Level II organisms (i.e., primary consumers), those that feed upon Trophic Level II organisms would be classified as Trophic Level III organisms (i.e., secondary consumers), and so on. This simple classification scheme is well recognized as a method to describe the flow of energy within the food web (e.g., see Parsons et al., 1977). The exchange and "flow" of PCBs within the system follows the same pathways as energy does (e.g., see Newman, 1998); thus, it is important to construct the modeling scheme using trophic level organization.

The organizational structure of the food web within the PRAM, where TL stands for trophic level, is presented in Figure 8 as follows:

- Pelagic Community: (open water organisms that spend the majority of their time and obtain the majority of their food in open water within both the upper and lower water column)
  - phytoplankton (TL-I); free-floating algae

conducted a fish consumption survey of local anglers, and estimated the fraction ingested (FI) term that relates to the potential fraction of fish caught from the ex-VERMILION that the anglers may ingest out of the total amount of fish they may consume per year (NEHC, 2004).

- zooplankton (TL-II); small organisms that graze on free-floating algae and suspended particles (e.g., copepods, krill)

- planktivores (TL-III); organisms (mostly fish) that prey primarily on zooplankton (e.g., herring, some snappers)

- piscivores (TL-IV); organisms (mostly fish) that prey upon fish (e.g., jacks)

- Reef Community: (reef-associated organisms that spend most of their time and obtain the majority of their food from the artificial reef)

  - attached algae (TL-I)

  - sessile filter feeders (TL-II); non-moving organisms attached to the sunken vessel that filter small organisms and suspended particles from the water column adjacent to the artificial reef (e.g., barnacles, bivalves)

  - invertebrate omnivores (TL-II); mobile invertebrates that fed on attached algae and other invertebrates (e.g., echinoderms, some crustaceans)

  - invertebrate foragers (TL-III); mobile (walking/crawling) invertebrates associated with the surface of the reef that prey upon planktivores, filter feeders, and attached algae (e.g., many crustaceans, echinoderms)

  - vertebrate foragers (TL-III); fish that prey predominantly on the reef epifaunal organisms such as the filter feeders and invertebrate foragers (e.g., trigger fish)

  - predators (TL-IV); organisms that prey upon fish and invertebrates associated with the reef (e.g., groupers, barracuda, morays, sharks)

- Benthic Community: (sediment-associated organisms that spend most of their time on or in and obtain most of their food from the sediment bed[25])

[25] Primary producers (autotrophs) are not expected to occur in the benthic community. Energy inputs to this community comes from the fallout of living and dead organisms from the upper and lower water columns.

- infaunal macroinvertebrates (TL-II); macroinvertebrates (i.e., larger than 0.5 mm) that live and feed within the sediment bed (e.g., polychaete worms)
- epifaunal macroinvertebrates (TL-II) (e.g., certain amphipods, echinoderms)
- foragers (TL-III) (e.g., crustaceans such as crabs and lobsters)
- predators (TL-IV) (flounder, flatfish, skates, rays, sea basses)

As with any classification scheme, not all items (i.e., animals) will fit neatly into the trophic scheme. One of the most significant issues for modeling is the progression of diets over the life stage within a given species, resulting in a change of trophic status as the animal ages.

It is important to note that the PRAM does not attempt to describe the reef trophic structure per se. Rather, it conservatively describes and tracks the accumulation and transfers of PCBs along trophic pathways. This is an important distinction to conceptualize and implement the modeling scheme. The PRAM food web construct is simplistic relative to the true trophic structure of an artificial reef and its associated communities, but fully functional for conservatively illustrating the movement and potential accumulation of PCBs in those organisms that may be consumed by people or relevant ecological receptors (i.e., functional for its end purpose–risk assessment). By focusing on the PCBs, the chemical-physical properties that control PCB environmental fate, and the subsequent potential exposure pathways, the community food web structure can be simplified without loss of the detail required to assure conservative risk estimates.

For example, certain parasites can be considered predators, some at the trophic level IV, but do they not represent a significant PCB transport mechanism. Inclusion of parasites may be relevant and important in developing a proper trophic dynamic model for the reef but is not required if the model focus is on the transport of PCBs.

A more significant example involves the reef-associated trophic level III consumers. There are many fish within this trophic level, separated by specific niche exploitations. Those species that feed extensively on the epifaunal reef organisms, such as the trigger fish, would be expected to more exposed to the PCBs as they leach out of the vessel and accumulate into the encrusted reef organisms. In contrast, the more mobile and generalist trophic level III organisms that forage away from the vessel (e.g., bigeye) would be less exposed, and as such, not as relevant as a more closely associated species such as the triggerfish.

Thus, not all species or even species assemblages (e.g., feeding guild) need be modeled in the PRAM to assure it's utility as a risk assessment tool. The artificial reef community is illustrated conceptually in the context of potential PCB exposures in Figure 8.

2.6.2 PRAM Food Web Community Structure

From a structural and functional perspective, the dynamics of the PRAM communities (and ecosystems in general) are regulated by components that fall into three fundamental trophic levels:

- Producers, or organisms that use radiant energy (sunlight) to manufacture organic matter (biomass) from inorganic chemicals – i.e., green plants that include algae and free-floating microscopic plant-like organisms (phytoplankton)
- Consumers, or organisms that feed on other organisms – i.e., animals that are classified as:
    1. Primary consumers (plant-eaters or herbivores)
    2. Secondary consumers (omnivores)
    3. Tertiary/quaternary consumers (carnivores)
    4. Consumers of dead, often partially decomposed biological tissue, and/or biological wastes (detritivores/scavengers)
- Decomposers, or organisms that convert dead biological tissue (detritus/ carrion) and biological waste materials into simpler organic molecules – i.e., bacteria and fungi

Although each might exist temporarily in isolation (e.g., in a lab culture), these fundamental categories of living organisms must all be represented in some combination to constitute a sustainable (self-perpetuating) ecosystem. The presence and abundance of species belonging to these fundamental levels is a product (under natural conditions) of the food web; the presence and abundance of one species in the food web may be controlled (limited) by the presence and abundance of another species. For example, primary producers (green plants) limit the numbers of herbivorous animals in the sense that the plants are the animals' primary food source. Because certain carnivores in turn feed predominantly on herbivores, the green plants also exert a certain degree of control (though indirect) on carnivore populations.

The following table summarizes the functional components of ecosystems, which are relevant to the prospective artificial reef:

Fundamental Trophic Level	Ecosystem-Specific Functional Group	Functional Group Category
Producers	unicellular plants	Algae, phytoplankton, and periphyton[26]
Consumers	herbivores	invertebrate herbivores vertebrate herbivores
	detritivores	invertebrate detritivores vertebrate detritivores
	omnivores	invertebrate omnivores vertebrate omnivores
	carnivores	first-order carnivores second-order carnivores
Decomposers	microbial decomposers	bacteria, fungi

The particular species will vary by community, but tend to be morphologically and physiologically similar within their respective functional group categories. Most consumers (animals) are relatively mobile, and comparatively much more complex organisms (both structurally and physiologically) than plants and microbes. Thus there is greater diversity, in the sense of higher taxonomic levels (especially genera, families, and orders), of consumer organisms than of the simpler organisms that function as producers and decomposers. For this reason, the functional group categories for consumers are defined broadly; a brief description of each is provided below, together with examples of the community forms, and relevancy in the context of PCB transfers within the food web.

2.6.2.1 Herbivores and Guild Representatives

Herbivores are those animals that consume only plants (the primary producers or Trophic Level I organisms). Herbivorous animals fall into Trophic Level II of the food web. In the context of the marine environment without the presence of vascular plants, the vast majority

[26] Vascular plants are not expected to represent a significant member of the expected reef or benthic communities at the proposed ex-ORISKANY Memorial Reef.

of herbivores are invertebrates. The following table (adapted from Adey and Loveland, 1991) is useful to identify the major groups of herbivorous invertebrates that may or may not be present within the communities modeled within the PRAM.

The feeding behaviors are the key element shown in the table below, for modeling purposes. Selective filtering, rasping and "cell sucking" appear to be the most representative for the entire group of invertebrates. In pelagic forms, selective filtering seems the most common feeding behavior. Rasping and filtering seem best to represent the group in terms of structure such as rock outcrops and potentially the sunken reef. The benthic invertebrates seem to focus on rasping and cell sucking. In terms of PCB transfers, the protozoans are thought to behave much like the algae (see Spacie et al., 1995; Connolly, 1991).

General Representative Marine Invertebrate Herbivores

Phylum	Class or Order	Frequency of Herbivory within Group	Example Common name	Example Species[27]	Example of Tissue Eaten	Mode of Feeding	Predominant Community
Protozoa	Several	Many	Amoeba	*Amoeba dudia*	Diatoms	Cytoplastic engulfing	All
Nematoda	Several	Many	Nematodes	*Dorylaimida*	Algae	Sucking of cell contents	Benthic

27 The examples may or may not be applicable to a specific reef community, but are presented as+ representative for the taxa, as adapted from Adey and Loveland (1991).

Phylum	Class or Order	Frequency of Herbivory within Group	Example Common name	Example Species[27]	Example of Tissue Eaten	Mode of Feeding	Predominant Community
Echinodermata	Echinoidea	Many	Sea-urchins	*Echinus esculentus*	Seaweeds	Rasping	Reef and Benthic
Mollusca	Amphineura	Virtually all	Chitons	*Ischnochiton ruber*	Algal turfs, corallines	Rasping	Reef and Benthic
Arthopoda	Copepoda	Most	Copepods	*Calanus*	Phytoplankton	Selective filtering	Pelagic
	Isopoda	Some	Slaters	*Ligia oceanica*	Seaweed	Chewing	Benthic
	Euphausiacea	Most	Krill	*Euphausia superba*	Phytoplankton	Selective filtering	Pelagic, Reef

This suggests that the significant pathways for PCB transfers within the pelagic invertebrate community will come from the filtering of algae from the water. For the reef invertebrates, PCB pathways will come from the rasping of attached algae on the sunken vessel, and rasping of benthic algae (if present) and/or consumption of algae falling out of the water column onto the sediment bed.

Larval fish that feed on phytoplankton, and some smaller adult fishes such as herring, who also feed heavily on zooplankton, are specific examples of vertebrate (fish) herbivores within the pelagic community. Most pelagic planktivores and larval fish snatch or grab individual planktors (raptorial feeding), but some species, such as herrings, are true filter feeders. In all cases, the algae diet occurs only during some of the fish's life history, or represents only a part of its diet, such that these fish are better classified as omnivores (an animal that consumes both plant and animal tissues).

A similar situation occurs within the reef community, where the parrot fish (*Scarids*), tangs (*Acanthurids*), and to a lesser extent, the damselfish (*Pomacentrids*), are thought to represent the vertebrate herbivores. Parrot fish are true grazers, while the tangs are better classified as browsers. The damselfish that are primarily herbivores tend to browse mostly on benthic algae attached to rocky outcrops. While the parrot fish eats a significant amount of attached algae, its diet also includes a large amount of coral. While coral contains a significant amount of symbiotic zooxanthellae cells (i.e., algae), the majority of coral tissue consists of animal tissue (i.e., *Coelenterata*). In this sense the parrot fish is not a "true" herbivore, but rather, is more akin to an omnivore.

Most tangs and surgeon fish graze on filamentous algae and typically reside in well-lit surge zones, where plentiful attached algae can be found, and can be considered true herbivores. Certain genera of the damselfishes (*Pomacentrids*) are known to be true herbivores, primarily associated with rocky bottoms and attached algae. Because of the sandy bottom and the depth of the ex-ORISKANY Memorial Reef site location, the presence of attached or benthic colony-forming algae (benthic algae) is considered unlikely. The overwhelming input of primary producer biomass to the benthic community is believed to be through fallout from the overlying surface waters, and not directly associated with any sediment bed substrate. As such, an herbivorous guild in the context of the benthic community is not considered to truly exist in the classical sense, and the "herbivores" present would be best represented by the invertebrate deposit and filter feeders (considered as detritivores in the next subsection).

The primary point of PCB entry into the biological food web from a sunken vessel is through the release to water and adsorption onto suspended particles and algae. The vast majority of fish within the pelagic zone that exhibit some herbivory do so as larvae. At this stage in life, many consider these fish as part of the macroplankton, or in the context of modeling PCB transfers, zooplankton. The inclusion of these fish within Trophic Level II is not necessary to trace the transfer(s) of PCBs from primary producers to, or through, Trophic Level II of the pelagic community food web, as they are accounted for within the zooplankton compartment of the PCB transfer model. Adult filter-feeding or particle-grabbing fishes, such as herring, are best characterized as omnivorous as they prey primarily on zooplankton and secondarily on algae. The foregoing suggests that, in the pelagic community, the zooplankton are the most appropriate group of organisms to trace PCB transfers from the primary producers into the pelagic food web.

The most significant primary producers directly associated with the reef community would be attached algae (colonial/filamentous). While floating algae may be present, water currents would relegate these organisms to more of a pelagic environment, such that the relevant PCB exposure would be associated with pelagic waters rather than reef waters, where the attached algae would reside.

Transfers from the reef community producers directly to true vertebrate herbivores are limited to species like the tangs. Tangs are poorly represented in the assemblages of reef fishes observed in and near the location of the proposed ex-ORISKANY Memorial Reef (Bortone et al., 1997). Of the reported 564 sampling events, *Acanthurins* (tangs) were observed 10 times (i.e., not quite 2% of the total number of samples) (Bortone et al., 1997). Only 20 individual fish were actually observed on and around the artificial reefs (Bortone et al., 1997). This suggests that while a true vertebrate herbivore population may be present at low density, the contribution towards any significant PCB transfer up to Trophic Level III or

IV due to predation is unlikely. Those predators present on the artificial reef would not receive a significant loading of PCBs from preying on a very small population of herbivorous vertebrates.

The most significant pathway for PCBs from the primary producers directly associated with the reef community would be through the grazing/foraging (mobile) invertebrate herbivores, such as urchins and mollusks.

2.6.2.2 Detritivores and Guild Representatives

Detritivores are animals that primarily consume dead biological tissue (carrion) or excreta. Most of the organisms that fit into this guild are benthic animals, but filter feeders on a reef feeding on suspended particles could be classified as detritivores as well, at least to some extent. Multiple macroinvertebrate taxa can be classified as detritivores, e.g., annelid worms, mollusks, and arthropods. To a certain extent scavenging organisms such as many crabs, shrimp, and some fish (e.g., hagfish, sharks, etc.) can also be classified as detritivores.

Detritivores that fall into the Trophic Level II or III position within the food web are relevant for the PRAM. Large carrion feeders, in the context of PCB modeling, effectively act as top predators, as their diet generally includes many Trophic Level III/IV animals. On the other extreme are the very small carrion feeders such as bacteria and other micro/macro invertebrates. Here in the context of PCB modeling, the biomass associated with the carrion of larger Trophic Level III/IV organisms is small relative to Trophic Level I or II biomass (e.g., see Parsons et al., 1977). This carrion PCB transfer pathway should be considered at the trophic III level to assure that the pathway is not “missed” in the model. Detritivores that fall within the Trophic Level II position must also be considered, and are best represented by deposit feeder and filter feeder guilds, in the sense of food web dynamics and biomass (e.g., Parsons et al., 1977; Adey and Loveland, 1991). In a general sense, many filter feeders are not true detritivores, given that they consume a significant amount of living material. However, for evaluating PCB transfers, given that part of their diets are known to include fecal pellets and seston, filter feeders can be used to represent the PCB transfers from detritus derived from lower trophic level carrion. It is important to note that the greatest mass of detritus/carrion is derived from Trophic Levels I and II biomass (e.g., see Parsons et al., 1977).

Within the pelagic community the detrital pathway can/should be accounted for utilizing zooplankton and/or planktivorous fish by adjusting their diets to include some detritus (as suspended particles representing Trophic Level I/II carrion) within their matrix.

Within the reef community the sessile filter feeders such as bivalves and barnacles would be expected to consume organic-rich suspended particles such as phytoplankton/zooplankton carrion along with live plankton. Mobile walking and/or crawling epifaunal species associated with a typical reef community, such as crustaceans (e.g., crabs and shrimps), are associated with carrion feeding. Such crustaceans are known to forage opportunistically, commonly ingesting carrion, living organisms, and even plant material. These crustaceans are probably more appropriately classified as omnivores than detritivores, and should be re-considered as omnivores or 1st order carnivores in the next subsections here. The most significant consumers of detritus derived from Trophic Level I and II organisms are the filter/ deposit feeders on the reef, as represented by bivalves and barnacles.

Within the benthic community the detritivores represent the largest biomass relative to all other guilds. Most of these detritivores are bacteria, fungi, microbenthos (<0.1 mm), meiobenthos (0.1 mm to 0.5 mm) and macrobenthos (>0.5 mm).[28] However, in the context of the transfers into the food web, other larger forms (the macrobenthos or macroinvertebrates with the micro and meiobenthos, hereafter referred to as microinvertebrates) represent the major predators or consumers of their community. These macroinvertebrates represent the transfer pathway out of the sediment bed and into the food web to top predator fish consumed by humans and/or relevant ecological receptors. Although microinvertebrates are far more numerous than macroinvertebrates per unit area, typically the biomass of macroinvertebrates is far greater than that of the microinvertebrates per unit area. For example, Parsons et al. (1977) report a study that revealed an overall abundance ratio of 1:70 for macrobenthos and meiobenthos, respectively in number of individuals, but a biomass ratio of 24:1 by fresh weight. Additional data collected from the scientific literature at that time (Parsons et al., 1977, Table 34) showed a consistently higher biomass for the macrobenthos, even if ciliates were considered over a significant range of geographical areas and sediment bed types in the ocean.

Two types of benthic (sediment-associated) macroinvertebrates are considered within the PRAM, infaunal and epifaunal forms. Infaunal refers to those macroinvertebrates that live *within* the sediment bed itself, whereas the epifaunal forms live *upon* the sediment bed (e.g.,

[28] Benthos classification after Levinton (1982) as cited in Adey and Loveland (1991).

see Parsons et al., 1977). There is significant overlap among the many species at issue here. Some species build tubes within the bed but feed from the sediment bed surface, while other tube builders will migrate into the water column to feed and return to their tubes for shelter from predation. Many of the epifaunal forms such as shrimp and scallops make extensive movements into the water column (e.g., see Parsons et al., 1977). By considering where maximum PCB exposure would or could occur, the relevant invertebrate forms can be identified.

Certain infaunal benthic forms, such as the true worms (annelids, i.e., the burrowing polychaete worms), do not build tubes nor do they migrate out of the sediment bed to any significant degree. They consume organic-rich sediment particles (detritus) that are coated with the bacteria and microinvertebrates, as discussed above. Clearly these benthic macroinvertebrate forms are significant in the context of PCB transfers from the sediment into the food web, as these organisms also represent a significant forage base for higher trophic level animals. To capture the transfer of PCBs into the detrital food web, infaunal macroinvertebrate worms are the best representative group of infaunal benthic organisms.

Epifaunal benthos include both macro- and mega-invertebrates, such as nudibrancs, echinoderms, mollusks, and crustaceans. The majority of these mega-invertebrates are predators and thus not relevant to detrital pathways, although many of the mollusks are filter or deposit feeders. As noted previously, the greatest input of biomass and energy into the detrital food web is derived from the pelagic primary producers and pelagic primary consumers. Thus, the most significant pathway to trace in order to follow the trophic transfers of PCBs is to identify the major consumers of this type of detritus. The epifaunal deposit and filter feeders represent the primary consumer guild in this context and as such, the relevant guild for tracing PCB transfers. Typical representatives include nematodes, polychaetes (deposit feeders) and bivalves (filter feeders).

2.6.2.3 Omnivores and Guild Representatives

Omnivores are animals that consume both plant and animal tissue, generally in a fresh state. For purposes of modeling the PCB transfers within the food web, however, consumption of carrion and detritus is considered relevant for this guild. There are many taxonomic representatives within this guild for both invertebrates and vertebrates. This guild, by definition, is between Trophic Level II (primary consumers) and Trophic Level III (secondary consumers).

As discussed above on the pelagic community, planktivores such as herring will consume floating algae as part of their diet. Additionally, there are invertebrates in the pelagic water column, such as species of shrimp that consume both algae and zooplankton. Consumption of dead algae and zooplankton has been identified as a potentially relevant and significant transfer pathway for PCBs. Given the low frequency in herbivorous species within the pelagic community and the fact that a diet consisting of algae and zooplankton (live or dead), in the context of PCB concentrations, will be lower than a diet strictly of zooplankton , the omnivore guild does not appear to be relevant for conservatively tracing the transfers and potential buildup of PCBs within the pelagic food web.

Within the reef community there are numerous examples of both vertebrate and invertebrate omnivores. The parrot fish, discussed previously, can be classified as an omnivore. Sea urchins, also mentioned earlier, consume significant quantities of algae, but also consume animal tissues. Many shrimps are also omnivorous. The representative detritivores identified as important in the context of PCB transfers, the filter feeders, are also in a sense omnivores. These filter feeders however, do not feed upon any attached algae directly associated with the sunken vessel, whereas organisms such as urchins and some crustaceans would. To capture the transfer of PCBs from attached algae, with the consideration of an elevated dietary PCB concentration due to additional consumption of hydroids, organisms such as urchins would represent a conservative pathway to trace.

The macroinvertebrates identified to represent the relevant PCB transport pathways within the benthic food web community consume detritus derived from both algae and zooplankton, as well as living forms of algae and zooplankton, and as such, are omnivores.

2.6.2.4 Primary (First Order) Carnivores and Guild Representatives

First order carnivores consume animals that are primarily herbivorous or in the case of the detrital food web, those detritivores that consume primarily detritus derived from algae and zooplankton. Organisms within this guild are considered to represent Trophic Level III within the PRAM.

Planktivorous fish are the primary group for consideration in modeling PCB transfers from Trophic Level II within the pelagic community. These animals consume mostly zooplankton, which represent the primarily consumers within the community, and represent a significant food source for higher trophic level predators.

While planktivorous fish would be expected to reside in the reef community as well, uptake into organisms such as filter feeders and urchins would be expected to represent the major PCB uptake pathway from lower trophic levels (filter feeders – see the discussion of detritivores, e.g., bivalves and rasping echinoderms such as urchins, see discussion of herbivores and omnivores). Both fish and other invertebrates will prey upon these organisms. Fish such triggerfish, and invertebrates such as crabs, are typical representatives for the predators of sessile filter feeders and crawling invertebrates such as urchins. Both of these types of predators forage along the reef. In addition, crabs will consume carrion, which was identified as a potentially relevant pathway for PCB transfers.

The infaunal and epifaunal macroinvertebrate detritivores, in the context of the PRAM benthic community food web (detrital food web), occupy Trophic Level II as primary consumers of detritus. Many organisms, both vertebrates and larger invertebrates, will prey upon these detritivores. Those predators in close proximity to the sediment bed that probe or sieve the sediment for these organisms would be expected to have a higher PCB exposure than those predators that capture the organisms as they move out of the sediment. Sediment probing and sieving predators of the macroinvertebrate detritivores include nudibrancs, crustaceans (e.g., crabs and lobsters), echinoderms, and skates, drums, and hogfish. Most fish, including those mentioned move extensively in the water column. The invertebrates, such as the nudibrancs, crabs, lobsters, and echinoderms, are in much closer contact with the sediment, and as such, are more likely to receive a higher exposure to any PCBs directly associated with the sediment than the more mobile fish or invertebrates such as squid. Thus, the most relevant first-order predators for tracing PCBs within the benthic community are those foraging invertebrates that probe or sieve the sediment for macroinvertebrate detritivores, such as the crustaceans.

2.6.2.5 Top (Second Order) Carnivores and Guild Representatives

Second order carnivores consume both herbivores and carnivores (and omnivores). These are top predators, and are classified as Trophic Level IV organisms.

The PRAM has been designed as a tool for human health risk assessment and as such, sports fish (primarily top predator fish) sought after and consumed by humans are the focus. The approach used in PRAM, as discussed above, has been taken to assure a conservative estimate of the transfer of PCBs into sports fish.

Within the pelagic food web, this trophic level is dominated by fish such as jacks, tuna, and sharks. Although some invertebrates, such as squid, could be considered to be at this level, they are generally not taken by recreational anglers. Of the typical pelagic fish taken by anglers, the jacks are perhaps the most representative given their, albeit slight, fidelity to structure.

Certain top predators on the artificial reef, such as eels and barracuda, are not commonly considered sports fish. Groupers are among the more popular sports fish on artificial reefs, and are top predators (Trophic Level IV).

A similar situation is present in the context of the benthic top predators, where organisms such as toadfish, skates, and sharks are true top predators; top predator fish such as the flatfish (e.g., flounder) are commonly sought and consumed by anglers. Other sport fish such as some snappers and sea bass forage extensively within the benthic community but return to the reef for shelter when not foraging. This will reduce their direct exposure levels to the sediment bed and in the context of PCB transfers decrease their overall exposure level, at least to the sediment-associated PCBs. To more clearly and conservatively characterize the potential transfers of PCBs from the sediment, these predators are not presently considered viable representatives.

2.6.3 Generalized Representative Dietary and Water Exposures for Use in Modeling PCB Food Web Transfers

This subsection summarizes the three PRAM communities – pelagic, reef, and benthic – in relation to the modeled food web, generalized trophic structure, assemblage guilds, and relevance to PCB transfers. Each discussion presents a "generalized" organism, along with a generalized diet and exposure profile, to characterize each trophic level within the food web. The approach discussed below, as implemented in PRAM, assures a conservative but plausible estimate of transfer of PCBs among the trophic levels within the food webs.

The PRAM does not attempt to model the trophic dynamics within and among the three biological communities but rather conservatively estimates the most efficient and significant pathways by which PCBs could accumulate to a "maximum" exposure level pertinent for risk assessment purposes.

2.6.3.1 Pelagic Community

The primary producers (Trophic Level I) within the pelagic community are the phytoplankton. The PRAM accounts for the fact that a pycnocline can/will form within the water column that will affect the dissolved PCB water concentrations. While algae may cross this boundary, they are not expected to remain as living cells but rather as falling particles, as the light attenuation with depth would limit algal growth and survival at depth. Thus, for algae, the relevant water exposure to PCBs is that concentration above the pycnocline, in well-lit waters.

In the context of abundance and ecological relevance within the pelagic community, the crustacean zooplankton represents the largest group, in terms of feeding habits and biomass, in most ocean waters (e.g., see Parsons et al., 1977), and as such, are the most relevant in considering the potential for accumulation of PCBs into Trophic Level II. Most of these zooplanktors are selective filter feeders that graze on the phytoplankton (e.g., Parsons et al., 1977). The dietary makeup for most of these zooplanktors is not well characterized in the sense of algae, bacteria, and/or particulate organic carbon but rather in a context of size. Considering PCB accumulation, bacteria, algae, and organic particulates are modeled as simple sorption materials (see Spacie et al., 1995; Connolly, 1991). The dietary breakout is not overly significant, except in the context of the relative sorption capacity of these dietary components. Within the PRAM this simplifies the available diet for this trophic level to suspended particles, which includes bacteria and suspended organic solids. The dietary breakout required for PCB food web modeling for a "generalized" Trophic Level II pelagic organism, as typified by crustacean zooplankton, is presented in Table 5, using copepods as the guild representative. Zooplankton are expected to migrate across this pycnocline and be exposed to PCB concentrations above and below the boundary. Feeding is expected to occur primarily in the upper water column where the phytoplankton are expected to be concentrated. Below the pycnocline only minimal feeding on suspended solids is predicted (Table 5).

Trophic level III pelagic planktivores (modeled as a herring-like fish) are assumed to feed exclusively on the zooplankton (Table 5). In reality, such fish are unlikely to feed exclusively on copepods, but as emphasized earlier, the PRAM is not designed to exactly mimic any true trophic dynamic structure, but rather, conservatively trace the potential accumulation and magnification of PCB concentrations along trophic pathways. Thus, the assumption of 100% zooplankton diet is used to assure that the planktivore (Trophic Level III) PCB concentration is not underestimated. Predation on the zooplankton will occur for most planktivores visually and as such, the water does not necessarily mirror that of the zooplankton but does assume a limited foray into the lower water column (80:20, Table 6).

In a similar vein, the top predator or Trophic Level IV animal (modeled as a jack-like fish) is assumed to feed almost exclusively (90%) on the planktivores (Trophic Level III) with a small fraction of the diet consisting of zooplankton (10%) to account for the ontogeny of diet over the fish's life stages (Table 5). This diet is in keeping with what has been reported for jacks (e.g., see Weaver et al., 2001). These predators are expected to follow the planktivores such that the predator water exposure regime mirrors the planktivores (80:20, Table 6).

2.6.3.2 Reef Community

The primary producers (Trophic Level I) directly associated with the artificial reef are attached algae. Given the depth of the ex-ORISKANY Memorial Reef, the presence of algae on the vessel will likely be limited to the upper portions of the prospective reef due to its radiant energy requirement. Nevertheless, these waters are predicted to be below the pycnocline. The water exposure level for attached algae is set as such (Table 6).

Two groups of primary consumers (Trophic Level II) are identified as relevant to assure a conservative estimate of PCB uptake through the reef community food web. The first group is the filter feeders, which are considered here to be sessile organisms (modeled as bivalves). Although Trophic Level II organisms are generally herbivores, in the context of a conservative evaluation of PCB transfers, omnivores are considered relevant and a conservative approach here. Bivalve mollusks and barnacles mostly feed upon algae with some suspended solids, but other filter-feeders on the prospective reef would feed on zooplankton (e.g., hydroids, etc.) as well. To reflect this fact, the filter feeder diet includes floating algae (80%), a fraction of zooplankton (10%), with a relatively small fraction of suspended solids (10%). This diet is not specific to any bivalve species, but rather, reflects the filter feeding community expected to occur on the artificial reef.

The second group of primary consumers (Trophic Level II) considered important for tracing PCBs through the reef community food web include omnivorous rasping echinoderms (modeled as an urchin). A generalized diet for these echinoderms emphasizes the herbivorous forms to reflect a Trophic Level II position and importance of the PCB transfer from attached algae into the reef food web (80% of diet), but also sessile organisms such as the hydroids (20% of diet, Table 5).

Because the reef is not expected to extend above the pycnocline nor are the modeled organisms expected to migrate across the pycnocline, Trophic Level II organisms would be exposed to that PCB concentration in the lower water column of the model system, and potentially waters within the vessel if the organism(s) used the vessel interior. The sessile filterers are unlikely to extend into the vessel interior to any significant degree given low flow (low oxygen level) and food availability. However, there is a distant possibility that more mobile sessile filters, such as the echinoderms, may use the vessel interior as a place of shelter from predation such that a fraction of the water interior to the vessel respired by these organisms is set at 20% to assure a conservative "loading" of PCBs into these animals (trophic level) and 80% of the lower water column below the pycnocline (Table 6).

Trophic Level III within the reef food web includes foraging invertebrates and fish. Carnivorous crustaceans (modeled as crabs) were identified as a relevant pathway for tracing PCB transfers within the reef community. Foraging crustaceans within the reef community would be highly opportunistic in their dietary preferences; what is presented reflects those dietary items identified as the most relevant PCB transfer pathways where the diet is comprised of 50% echinoderms (reef food web Trophic Level II omnivores), 35% bivalve filter feeders (reef food web Trophic Level II filter feeders), and to account for a limited input from the pelagic community as infrequent visitation and/or as carrion (considered a potentially significant PCB transport pathway) 5% zooplankton, 5% pelagic planktivorous fish, and 5% suspended solids (sorption materials, including bacteria, organic matters, and detached algae). The relevant vertebrate (fish) forager representing Trophic Level III within the reef community would have a diet again of those organisms that were identified as salient for a conservative trace of PCBs transport, the sessile filter feeders (modeled as bivalves) and invertebrate omnivorous foragers (modeled as urchins). For this type of fish (modeled as trigger fish), the dietary components include some planktivorous fish (19%) as well as the aforementioned reef carnivorous invertebrate foragers (22%), modeled as a crab, omnivorous echinoderms (15%), modeled as an urchin, sessile filter feeders (19%), modeled as bivalves, epifaunal benthos (12.5%), and infaunal benthos (12.5%) (Table 5). This dietary breakout is in keeping with reports for the gray trigger fish (e.g., see Nelson and Bortone, 1996), and the TWG recommendations. Both the foragers (Trophic Level III reef carnivores) are assumed to be present only within the reef community and as the prospective reef will be below pycnocline, water exposure would be of the water PCB concentration within the lower water column and/or water interior to the sunken vessel as used for potential shelter from predation (Table 6). The percentage of vessel interior respired waters (30%) is slightly higher than that for the echinoderm omnivores (20%) due to the behavior associated with these predators (i.e., more time spent resting in nooks and crannies along the artificial reef than foraging omnivores such as urchins).

A top reef predator consumes primarily Trophic Level III organisms from off the reef. Not all top predators that reside on the reef prey exclusively on reef organisms. For example, the gag grouper, while considered to be a reef resident, preys heavily on pelagic planktivorous fish. When tracing PCBs from the reef into sports fish, the diets of a species such as the gag grouper cannot be considered conservative. To assure a degree of conservatism and to maintain the logic train of following PCBs within each food web, the top reef predator (Trophic Level IV) is assumed to prey primarily (60%) on reef Trophic Level III fish (modeled as trigger fish) and Trophic Level III invertebrates (15%) (modeled as crabs) (Table 5). As these top predators have less need for shelter the relative exposure to the interior vessel water concentrations of PCBs is reduced relative to Trophic Level III reef organism (Table 6) but still assumed to remain on the reef and thus not be exposed to the PCB water concentrations in the upper water column.

2.6.3.3 Benthic Community

No primary producers (Trophic Level I) are expected to occur along the sediment bed associated with the ex-ORISKANY Memorial Reef due to the depth of the water and light attenuation at that depth.

Two types of macroinvertebrate detritivores (Trophic Level II) organisms were identified as relevant for following PCBs moving onto the detrital (benthic) food web, infaunal and epifaunal animals. The infaunal organisms (modeled as polychaetes) that burrow into and reside within the sediment bed are assumed to consume sediment that is coated with bacteria and microbenthos associated with the sediment particles. The diet of these organisms is represented in Table 5 where the animals consume 50% sediment particles, 30% algal cells and 20% zooplankton that have fallen from the water column. Here again this diet is developed in a context of the general group of burrowing worms and recognizes that the direct transfers from the sediment (a PCB sink within the model system) are the most important to assure a conservative estimate of exposures. The epifaunal macroinvertebrates (modeled as nematodes) are represented as primarily deposit feeders with representative predators (e.g., *Euncida* and *Phyllodocida*) of other worms and small infaunal organisms with a fractionated diet made up of 25% sediment, 30% deposited algae, 20% deposited zooplankton, and 25% infaunal macroinvertebrates to reflect benthic predators within this guild (Table 5).

Considering the accumulation of PCBs from the water for the benthic food web Trophic Level III (infaunal and epifaunal macroinvertebrates), the exposure to sediment pore water is germane. The sediment pore water concentrations of PCBs may be higher than the concentration in the overlying water due to desorption for the sediment particles and diffusive impedance from the pore water into the overlying waters. In modeling the transport of PCBs, the infaunal macroinvertebrate, for the most part, rarely move into the overlying water but this is not to say they do not respire overlying waters (e.g., see Chapman et al., 2002), thus the relative water exposures for this group of animals is set conservatively at 80% pore water and 20% overlying surface water below the pycnocline (Table 6). The epifaunal macroinvertebrates live at the interface between the surface water and the sediment such that they respire predominantly overlying water. Nevertheless during feeding and disturbing the sediment bed, they would have a significant potential for pore water exposure, thus, to maintain a level of conservatism, the fractional water exposure for PCB accumulation via respiration is set at 50% pore water PCB concentrations and 50% surface water (below the pycnocline; see Table 6).

The relevant first order carnivores within the benthic community (Trophic Level III) in the context of maximal exposure levels are those that forage directly on the sediment and dig, probe of sieve the sediment for their prey. Among this group are organisms that are directly consumed by humans such as crabs and lobsters. Recognizing this and the objective for the PRAM (human health risk assessment), the lobster is a logical choice to represent this guild as well as provide for input into a risk assessment. The diets of lobsters includes mostly epifaunal macroinvertebrates such as gastropods, echinoderms, and bivalves (e.g., see FMRI, 2003). To maximize the potential transfer of PCBs, the lobster's diet (Table 5) is assumed to be composed of approximately an equal distribution of infaunal (50%) and epifaunal (45%) organisms and that the animal will incidentally consume sediment as it digs or probes into the sediment for these prey items (5%). Exposure to pore water concentrations of the PCBs would also be expected as this guild of animals (as represented by the lobster) forages along the sediment bed. To account for this exposure while recognizing that most of the water respired by an animal above the sediment will be of overlying water, the fraction of pore water respired is 25% of the total with 75% of the water respired being at the PCB concentration of the lower water column (Table 6).

Top predators within the benthic community include rays or skates, sharks, flatfish, toadfish, certain species of snappers, and others. Of note here are the sports fish that may be sought after and consumed by humans. Those organisms that feed heavily on Trophic Level III benthic guilds (modeled as the lobster) would be exposed to the highest concentration of PCBs. Such species would be more akin to sharks, skates, and rays. However, these are not the more common sports fish such as flat fish (e.g., flounders). Trophic level IV fish feeding on the sediment that would be expected to see the highest PCB concentrations in their diet would be those that feed heavily on the Trophic Level III benthic organisms (modeled as lobsters) and/or the sediment associated macroinvertebrates Trophic Level II invertebrates). Thus a dietary makeup of 58% Trophic Level III carnivores, 20% epifaunal macroinvertebrates, and 20% infaunal macroinvertebrates represents a reasonably conservative dietary exposure to assure that PCB tissue concentrations are not underestimated. As these top predators would capture their prey on and in the sediment bed, an incidental sediment ingestion of 2% is considered warranted again, to assure that the final tissue concentration of PCBs is not underestimated (Table 5). As these fish (modeled as a flounder) would be expected to be in close contact with the sediment while feeding and resting, they would be expected to be exposed to some level of higher PCB concentrations in the water. To account for these increased exposure concentrations the Trophic Level IV benthic predators are assumed to respire 10% sediment pore water and 90% water below the pycnocline (Table 6).

2.7 PRAM PCB TROPHIC TRANSFER METHODS AND ALGORITHMS

Several food web modeling schemes employing the fugacity concept have been developed for aquatic systems but all require a fairly reasonable estimate of the mass and volume of biological tissue present in the system. To avoid the assumption of a “typical” reef-based biomass or requiring user inputs of a variety of reef biomass scenarios, the PRAM was designed using thermodynamic equations, which at steady-state do not require total biomass estimates. Additionally, the model structure being based in bioenergetics is more directly and explicitly affected by system temperature and dissolved oxygen than a model structured by fugacity, which seems more desirable if one was to evaluate different climates for reef building. This is considered to be a conservative approach as the amount of PCBs is assumed to be unlimited in the system where no decrease in PCB concentrations in water or sediment is assumed to occur as a consequence of the accumulation into biological tissue.

Bioconcentration of PCBs by aquatic organisms from *water* can be described as a one-compartment, first-order kinetics model (e.g., see Equation 10 in Spacie and Hamelink, 1995; Equation 3.19 in Newman, 1998):[29]

$$(93)\ \frac{\Delta C_i}{\Delta t} = \text{uptake - loss} = \left(Ku_i \left[\frac{L}{kg_{lp} \cdot d} \right] \times C_w \left[\frac{mg}{L} \right] \right) - \left\{ \left(Ke_i \left[\frac{1}{d} \right] + G_i \left[\frac{1}{d} \right] \right) \times C_i^t \left[\frac{mg}{kg_{lp}} \right] \right\}$$

where:

ΔC_i	=	change in tissue concentration for organism *i* [mg/kg_{lp}]
Δt	=	change in time [days]
Ku_i	=	uptake rate constant for water in organism *i*
C_w	=	concentration of PCB in water (surface water and/or sediment pore water)
Ke_i	=	elimination rate constant (sum of elimination and metabolism) for organism *i*
G_i	=	growth rate for organism *i*
C_i^t	=	PCB concentration in organism *i* at time *t*
kg	=	kilogram
mg	=	milligram
L	=	liter
d	=	day
lp	=	lipid [30]

Uptake and accumulation of PCBs by aquatic organisms from *food* can also be described with a simple one-compartment, first-order kinetics model (e.g., see equation 34 in Spacie and Hamelink, 1995; equation 3.24 in Newman, 1998):

$$(94)\quad \frac{\Delta C_i}{\Delta t} = \alpha\ I_{i,j} \left[\frac{1}{d} \right] C_j \left[\frac{mg}{kg_{lp}} \right] - \left\{ \left(Ke_i \left[\frac{1}{d} \right] + G_i \left[\frac{1}{d} \right] \right) \times C_i^t \left[\frac{mg}{kg_{lp}} \right] \right\}$$

where:

ΔC_i	=	change in tissue concentration for organism *i* [mg/kg_{lp}]
Δt	=	change in time [days]

[29] Spacie and Hamelink (1995) combine the two loss terms (Ke and G) as a first order rate constant for depuration denoted as K_d.

α = assimilation efficiency of COC across digestive tract of organism *i* [fraction]

$I_{i,j}$ = ingestion rate of dietary item *j* for organisms *i*

$kg_{lp\cdot j}/kg_{lp\cdot i}$ = kilogram lipid of dietary item *j* consumed per kilogram lipid of organism *i*

C_j = COC concentration in the dietary item *j*

Ke_i = elimination rate constant (sum of elimination and metabolism) for organism *i*

G_i = growth rate for organism *i*

C_i^t = COC concentration in organism *i* at time *t*

Equation 94 can be combined with Equation 93 to estimate tissue concentrations of aquatic organisms contributed via water, sediment, and food assuming that a "steady-state"[31] condition has been reached and, as such, the change in chemical concentration (lipid-based) over time becomes zero. At equilibrium, the rate at which the chemical enters the organism and the rate at which the chemical is eliminated or metabolized are balanced. Equation 94 assumes only one dietary item, which for the aquatic animals within the PRAM is not appropriate. To account for multiple dietary items, Equation 94 is modified and combined with Equation 93 as follows:

$$(95)\quad \frac{\Delta C_i}{\Delta t} = 0 = \left(Ku_i \times C_w\right) + \sum_{j=1}^{n}\left(\alpha I_{i,j} C_j^{ss}\right) - \left[\left(Ke_i + G_i\right) \times C_i^{ss}\right]$$

where:

ΔC_i = change in tissue concentration for organism *i*

Δt = change in time (days)

Ku_i = uptake rate constant for water in organism *i*

C_w = concentration of PCB in water (surface water and/or sediment pore water)

α = assimilation efficiency of PCB in dietary item *j* across digestive tract of organism *i*

$I_{i,j}$ = ingestion rate of dietary item *j* by organism *i*

C^{ss}_j = concentration of PCB in dietary item *j* at thermodynamic steady-state

[30] All concentrations are normalized by lipid content in keeping with the approach presented by Thomann (1981) and others.

[31] Thermodynamic equilibrium, or "steady-state," is defined as when uptake and loss are balanced such that the change in tissue concentration is zero, as depicted in Equation 95.

Ke_i = elimination rate constant (sum of elimination and metabolism) for organism *i*
G_i = growth rate for organism *i*
C^{ss}_i = concentration of PCB in organism *i* at thermodynamic steady-state
n = number of dietary items
j = specific dietary item *j*

Equation 95 is equivalent to the governing equation(s) used by Gobas (1993), Connolly (1991), and Thomann et al. (1992). As described above, the first term represents the direct uptake of PCB by the animal from water, the second term represents the flux of PCB into the animal through feeding, and the third term is the loss of PCB due to metabolism and excretion plus the change in concentration due to growth.

According to Spacie et al. (1995) and others, the uptake of chemicals (i.e., PCBs) into aquatic animals should be based on the "freely dissolved"[32] fraction of the chemical in water. Given the organic carbon (oc) fraction and the particulate organic carbon content in the water column (f_{oc}) can be calculated. Spacie et al. (1995, Equation 9) provides the following equation from which a freely dissolved water concentration can be derived:

$$(96) \quad C_{dw} = \frac{C_{tw}}{1 + f_{oc} \times K_{oc} + f_{doc} \times K_{doc}}$$

where:
C_{dw} = freely dissolved COC concentration in water
C_{tw} = total COC concentration in water
f_{oc} = fraction of particulate organic carbon within the water column
K_{oc} = organic carbon-water partition coefficient
f_{doc} = fraction of dissolved organic carbon within the water column
K_{doc} = dissolved organic carbon-water partition coefficient

The fraction freely dissolved PCB concentration = $f^{fd} = \frac{C_{dw}}{C_{tw}}$

Therefore,

[32] Freely dissolved refers to the total concentration of a PCB in surface water minus that fraction adsorbed to suspended particulate organic carbon and dissolved organic carbon (see Spacie et al., 1995; USEPA, 1995).

$$(97) \quad f^{fd} = \frac{1}{1 + \left(f_{oc}\left[\frac{kg}{L}\right] \times K_{oc} \right) + \left(f_{doc}\left[\frac{kg}{L}\right] \times K_{doc} \right)}$$

where:

f^{fd}	=	fraction of PCB concentration that is freely dissolved
f_{oc}	=	fraction of particulate organic carbon within the water column
f_{doc}	=	fraction of dissolved organic carbon within the water column
K_{oc}	=	organic carbon – water partition coefficient
K_{doc}	=	dissolved organic carbon – water partition coefficient

2.7.1 Equations that Describe Food Transfers of PCBs

Estimates of uptake and accumulation of PCBs from the diet of aquatic animals requires a description of the food web or food chain within which the PCBs are interacting. As described above, the food web within the PRAM consists of three inter-related communities: the benthic (sediment bed-associated), reef-associated (vessel-associated), and pelagic (water column-associated) communities.

As previously described, PCBs will enter the food web via uptake across the respiratory tissues of aquatic animals and across the digestive tract of those animals that consume organic carbon within the sediment (bedded or suspended in the water column) as an energy source. These PCBs can then be transferred within the food web via consumption of aquatic biota (e.g., from aquatic worms feeding on sediment into bottom foraging fish or other invertebrates). If the accumulation of PCBs is highly efficient, but the depuration rate is low (i.e., not readily excreted or metabolized), the relative concentrations of the PCB among the trophic levels depicted above can become significantly elevated along the food chain. This phenomenon is commonly referred to as biomagnification (e.g., see Newman, 1998).

Biomagnification is quantified within PRAM by the calculation of two separate factors, the bioconcentration factor (BCF) and the bioaccumulation factor (BAF). Both factors represent the ratio between the PCB concentration in the organism's tissues and the PCB concentration in the water. The difference between the factors is in the source of the PCBs; the BCF represents only the PCBs collected directly from the water, while the BAF represents PCBs collected from water plus PCBs collected from food (and therefore includes an organism's BCF as one of its components).

The governing equation (Equation 95) was developed specifically to describe the movement of organic chemicals such as PCBs within an aquatic food chain (Thomann, 1981, 1989; Connolly, 1991; Thomann et al., 1992). The following sections describe how Equation 95 was adapted to describe the movement of PCBs in the PRAM by extension to the ex-ORISKANY Memorial Reef.

2.7.1.1 Bioconcentration Factors

BCFs represent the PCBs taken by an organism directly from the water, and therefore do not include food sources. Restating equation 95 without the food sources, we have the steady-state concentration of PCBs contributed directly from the water:

$$(98)\quad \frac{\Delta C_i}{\Delta t} = 0 = \left(Ku_i \times C_w\right) - \left[\left(Ke_i + G_i\right) \times C_i^{ss}\right]$$

We can then solve for the BCF as follows:

$$(99)\quad BCF_i\left[\frac{L}{kg_{lp}}\right] = \frac{C_i^{ss}}{C_w} = \frac{Ku_i\left[\dfrac{L}{kg_{lp}\cdot d}\right]}{Ke_i\left[\dfrac{1}{d}\right] + G_i\left[\dfrac{1}{d}\right]}$$

Equation 99 is utilized in PRAM to calculate the BCF of all organisms except the trophic level I primary producers (algae). Algae (free floating or attached to the sunken vessel) are assumed to act primarily as sorption material for PCBs freely dissolved in the water column. As such, the concentration within algae is dependent on the adsorbent (lipid) concentration within the algae, which can be directly related back to the PCB's octanol-water partition coefficient (K_{ow} – e.g., see Thomann, 1989). However, for chemicals with a $\log K_{ow}$ greater than 5.0, the algal BCF becomes constant (see Spacie et al., 1995; Connolly, 1991):

$$\begin{aligned}&if\ \log K_{ow} \le 5.0\\&then;\\&BCF_{ag}\left[\frac{L}{kg_{lp}}\right] = K_{ow}\\(100)\quad&\\&if\ \log K_{ow} > 5.0\\&then;\\&BCF_{ag}\left[\frac{L}{kg_{lp}}\right] = 10^5\end{aligned}$$

where:

BCF_{ag} = bioconcentration factor for algae (*ag*) exposed to freely dissolved PCB water concentrations

K_{ow} = octanol-water partition coefficient

The floating algae are considered to be solely exposed to PCBs dissolved in the water above the pycnocline (C_{wu}) whereas attached algae on the sunken vessel are assumed to be exposed solely to PCBs dissolved in the water below the pycnocline (C_{wl}).

2.7.1.2 Tissue Concentrations

The concentration of PCBs in an organism's tissue is derived from Equation 95 and utilizes the BCF term calculated in Equation 99. First, Equation 95 is solved for the steady-state concentration of PCBs in tissue:

$$(101)\ C_i^{ss} = \frac{Ku_i \times C_w}{Ke_i + G_i} + \frac{\sum_{j=1}^{n}\left(\alpha I_{i,j} C_j^{ss}\right)}{Ke_i + G_i}$$

Substituting the BCF from Equation 99 into Equation 101 we have the governing equation for calculation of tissue concentrations in PRAM:

$$(102)\ C_i^{ss}\left[\frac{mg_{PCB}}{kg_{lp}}\right] = BCF_i\left[\frac{L}{kg_{lp}}\right] \times C_{w,i}\left[\frac{mg_{PCB}}{L}\right] + \frac{\alpha[unitless]}{\left(Ke_i\left[\frac{1}{d}\right] + G_i\left[\frac{1}{d}\right]\right)}\sum_{j=1}^{n}\left(I_{i,j}\left[\frac{1}{d}\right]C_j^{ss}\left[\frac{mg_{PCB}}{kg_{lp}}\right]\right)$$

where:

$C_{w,i}$ = weighted average of all water concentrations to which organism i is exposed

For Trophic Level I primary producers, who consume no other organisms (n = 0), this equation is a function of only the water concentration and the BCF_{ag} term presented in equation 100. For all other organisms, the tissue concentrations of the prey organisms they consume must be computed first and entered into equation 102.

In Equation 102, it is necessary to utilize a weighted average of all PCB water concentrations to which an organism is exposed since most species spend their time in multiple compartments with different water concentrations. For example, most pelagic species spend time both above and below the pycnocline. The weighted average is calculated from the fraction of time spent in each compartment as follows:

$$(103)\ C_{w,i}\left[\frac{mg_{PCB}}{L}\right]=\sum_{c=1}^{n}\left(f_{c,i}\left[unitless\right]\times C_{w,c}\left[\frac{mg_{PCB}}{L}\right]\right)$$

where:

c = compartment of unique water concentration (above pycnocline, below pycnocline, inside vessel or sediment pore water)

n = number of compartments to which an organism is exposed

$f_{c,i}$ = fraction of time organism i spends in compartment c

$C_{w,c}$ = concentration of PCBs in water of compartment c

Since all tissue concentrations in PRAM are calculated on a lipid-normalized basis, the concentrations of the PCB homologs in the whole organism are calculated from equation 102 as follows:

$$(104)\ C_{ww,i}^{ss}\left[\frac{mg_{PCB}}{kg_{ww}}\right]=C_{lp,i}^{ss}\left[\frac{mg_{PCB}}{kg_{lp}}\right]\times f_{lp,i}\left[\frac{kg_{lp}}{kg_{dw}}\right]\times\left(1-f_{moist,i}\right)\left[\frac{kg_{dw}}{kg_{ww}}\right]$$

where:

$C^{ss}_{ww,i}$ = steady-state concentration of PCBs in whole organism i

$C^{ss}_{lp,i}$ = steady-state concentration of PCBs in lipid tissue of organism i (C^{ss}_{i} term from equation 102)

$f_{lp,i}$ = fraction of lipids in dry tissue of organism i (see Table 7)
$f_{moist,i}$ = fraction of water in organism i (see Table 7)

2.7.1.3 Bioaccumulation Factors

BAFs are similar to BCFs since they both represent the ratio between the PCB concentration in the organism's tissue and the PCB concentration in the surrounding water; however, the BAFs represent the PCBs contributed to the organism's tissues by both the surrounding water and the food eaten by the organism. By including both major PCB sources, the BAF term serves as an indicator of the total PCB accumulation in the organism's tissues. PRAM calculates BAFs directly by utilizing the lipid-based tissue concentrations from Equation 102 and the average water concentrations from Equation 103:

$$(105)\ BAF_i\left[\frac{L}{kg_{lp}}\right] = \frac{C_i^{ss}\left[\frac{mg_{PCB}}{kg_{lp}}\right]}{C_{w,i}\left[\frac{mg_{PCB}}{L}\right]}$$

2.7.2 Derivation of Rate Constants

The concentrations of the various food web components described above are all based on either a wet-weight or lipid-weight basis. To convert to either a lipid-based or a dry weight-weight basis, values presented in Table 7 are used.

The algorithms previously described are based on thermodynamic kinetics and, as such, require rate constants. Specifically these rate constants include:

- Ingestion rates and dietary assimilation efficiencies.
- Growth rates.
- Uptake rate constants and assimilation efficiencies for water exposure.
- Elimination and metabolism rate constants.

2.7.2.1 Oxygen Consumption Rates, Dietary Ingestion Rates, and Bioenergetics

To estimate the dietary ingestion rates and growth rates for the animals within the PRAM, daily energy (calorie) requirements are calculated based on oxygen consumption. The total energy consumption, or maintenance energy budget (energy in = energy out), of an organism is described by the following relationship (e.g., see Jobling, 1994 and Welch, 1968):

$$(106)\ Cn\left[\frac{kcal}{d}\right] = G\left[\frac{kcal}{d}\right] + R\left[\frac{kcal}{d}\right] + F\left[\frac{kcal}{d}\right] + U\left[\frac{kcal}{d}\right]$$

where:
Cn = metabolic energy consumption of the organism
G = metabolic energy usage for production (i.e., growth and reproduction) – not to be confused with the growth rate (G) term presented in Equations 93 – 95
R = metabolic energy usage by tissues (derived from respiration)
F = energy loss due to fecal excretion
U = energy loss due to urinary excretion
d = day
kcal = kilocalories

The ingestion rate of an aquatic animal must meet these energy requirements to survive. Welch (1968) and Parsons et al. (1977) provide the energy budgets for aquatic animals [note that Welch (1968) combined energy loss due to fecal (F) and urinary (U) excretion as total excretion (EX)] as presented in Table 7. Using the energy budget, oxygen consumption rates can be used to estimate metabolic rates, which in turn can be used to estimate food ingestion rates (e.g., see USEPA, 1993).

Oxygen consumption rates are temperature-dependent and weight-dependent in aquatic animals, and can be calculated using allometric regressions derived from experimental data (see Connolly, 1991; Altman and Dittmer, 1971; Hewett and Johnson, 1992; USEPA, 1993, Barber, 2003; Thurston and Gehrke, 1993; and Kline, 2004). PRAM respiration rates are based upon the equation presented by Connolly (1991, Equation 10), which calculates respiration as a metabolic rate with units of (day^{-1}). Except for benthic foraging invertebrates, represented by the lobster, respiration for all invertebrate compartments in the food web is based solely on temperature and normalized to body weight. For these species the β_1 term in Equation 107 is zero. All of the vertebrate compartments within the food web, and the benthic foraging invertebrate, are represented by a regression that includes a weight as well as temperature component. For these species the β_1 term in Equation 107 is non-zero. The governing equation for respiration of all species is:

$$r\left[\frac{1}{day}\right] = \alpha W[g]^{\beta_1} e^{\beta_2\left(T\left[^oC\right]\right)} \tag{107}$$

where:

r = oxygen consumption rate (1/day)
W = organism body wet weight in grams (g)
T = temperature (degrees Celsius)
α = allometric intercept
e = the base of the natural logarithm
β_1, β_2 = allometric slopes for body weight and temperature, respectively

PRAM uses direct respiration rates with units of gO_2/kg_{lp}-day; therefore, the rate provided by Equation 107 must be converted from a metabolic rate. The conversion is done by using the three factors presented in Equation 108: a_{oc}, a_c, and f. Values for a_{oc} and a_c have been obtained from Thomann (1989). The conversion has been calculated in PRAM as follows where the subscript *i* represents organism *i*:

$$r'_i\left[\frac{gO_2}{kg_{lp}\cdot d}\right] = r\left[\frac{1}{day}\right] \times \frac{a_{oc}\left[\frac{gO_2}{gC}\right] \times a_c\left[\frac{gC}{g_{dw}}\right] \times \left(\frac{1000 g_{lp}}{kg_{lp}}\right)}{f_{lp,i}\left[\frac{g_{lp}}{g_{dw}}\right]} \tag{108}$$

where:

r'_i = oxygen consumption rate (gO_2/kg_{lp}-day)
gO_2 = oxygen (gm)
kg_{lp} = mass of lipids in fish (kg)
a_{oc} = stoichiometric oxygen/carbon ratio (2.67 gO_2/gC for all species)
a_c = fraction of carbon in dry weight (0.45 gC/g_{dw} for all species)
$f_{lp,i}$ = fraction lipids in dry tissue of organism *i* (see Table 7)

Allometric intercepts and slopes have been compiled or derived from the peer-reviewed scientific literature for the food web compartments and are presented in Table 8 and Appendix E.

Rather than calculating metabolic energy consumption rates or food ingestion rates directly from Equation 106, they can instead be estimated from respiration metabolic rates based on kilocalories. The oxygen consumption rates developed from Equation 108 are converted to a kilocalories basis (Equation 109) using: (1) the molar volume of oxygen under average site conditions,[33] and (2) an approximate conversion factor of 4.8 calories = 1 mL of O_2 (USEPA, 1993). The overall metabolic energy consumption rate is then estimated from the respiration metabolic rate by dividing by the fraction of metabolism dedicated to respiration:

$$(109)\ Cn_i\left[\frac{kcal}{kg_{lp}\cdot d}\right]=\frac{r_i^{'}\left[\frac{gO_2}{kg_{lp}\cdot d}\right]\times\frac{1mLO_2}{0.00131gO_2}\times\frac{0.0048kcal}{1mLO_2}}{f_{resp,i}}$$

where:

$f_{resp,i}$ = fraction of organism's energy budget devoted to respiration (see Table 7). Per Welch (1968), the energy budget (Equation 106) can be thought of as fractions where Cn = 1 and each energy component is less than 1.

To calculate the respective oxygen consumption rates for each of the food chain organisms, temperature and body weights are required. Additionally, since the goal is to first estimate the ingestion rates of the animals within the food chain model on a mass basis, caloric densities of prey organisms are required and are presented along with body weights in Table 7.

For example, assuming a lower water column temperature of 19.5°C, the following respiration rates and total energy consumption estimates are calculated for flounder:

(110)

[33] At standard ambient temperature and pressure (SATP; 25°C and 1atm), the molar volume of an ideal gas equals 24.47L. Therefore, there are 4.087×10^{-5} moles per mL of an ideal gas at SATP. Given the molecular weight of O_2 (~32g/mol), there are 0.00131g of O_2 per mL O_2 at SATP.

$$r_{flounder}\left[\frac{1}{day}\right] = 0.0046(3000)^{-0.24} e^{(0.067\times 19.5)} = 0.00249\ day^{-1}$$

$$r_{flounder}'\left[\frac{gO_2}{kg_{lp}\cdot d}\right] = 0.00249\ day^{-1} \times \frac{2.67\times 0.45\times 1000}{0.22} = 13.58\frac{gO_2}{kg_{lp}\cdot d}$$

$$Cn_{flounder} = \frac{\dfrac{13.58\, gO_2}{kg_{lp}\cdot d}\times\dfrac{0.0048}{0.00131}}{0.6} = 82.9\frac{kcal}{kg_{lp}\cdot d}$$

2.7.2.2 Total Energy Consumption and Ingestion Rates

To convert energy consumption to a mass ingestion rate requires converting food calories to food mass:

$$(111)\ I\left[\frac{kg_{lp}}{kg_{lp}\cdot d}\right] = \frac{Cn\left[\dfrac{kcal}{kg_{lp}\cdot d}\right]}{\left(\lambda\left[\dfrac{kcal}{kg_{lp}}\right]\times AE\right)}$$

where:

I = mass ingestion rate (i.e., kg_{lp} food / kg_{lp} body weight /day)

C_n = caloric ingestion rate

λ = caloric density of food item

AE = assimilation efficiency or fraction metabolizable calories of food item

To estimate the caloric content of sediment and suspended sediment within the system and consumed by filter feeders and other detritivores, the composition of the sediment and its edible fraction (detritus) need to be considered. In littoral zones, flowing rivers, and wetlands, detritus is primarily composed of vascular plant material, while in estuaries, bays, and the open ocean, detritus is derived largely from algae (e.g., see Mason and Varnell, 1996; Valiela, 1995; Parsons et al., 1977). Caloric content of salt marsh bulrush ranges from 3.2 kcal/g-dry weight to 4.8 kcal/g-dry weight (USGS, 2002), which compares well with the "aquatic" vascular plant caloric contents as reported by USEPA (1993), 4.0 to 4.3 kcal/g-dry weight. Algae are reported to have a much lower caloric content (2.36 kcal/g-dry weight;

USEPA, 1993). For the artificial reefs, the conservative assumption is made that the detritus present is derived from algae. According to Mason and Varnell (1996), the half-life for the decomposition of plant material in a salt marsh ranges from 18 to 350 days depending on the local conditions. To assure a level of conservatism, the detritus present is considered to be at 50% of its original caloric content as algae or 1.18 kcal/g-dry weight (1,180 kcal/kg-dry weight).

Given a dry-weight lipid content for algae of 0.103 kg-lipid/kg-dry weight (Table 7), the caloric content of sediment-associated detritus within the PRAM is approximately 11,456 kcal/kg-lipid (1,180 kcal/kg-dry weight ÷0.103 kg-lipid/kg-dry weight). It is further assumed that one-kilogram of lipid is equivalent to one-kilogram of organic carbon (Thomann et al., 1992 and others); thus the caloric content of organic carbon in the sediment is estimated to be 11,456 kcal/kg-organic carbon.

On a lipid basis, total ingestion is expressed by denoting each dietary preference as a fraction of the total diet as f_{diet} (decimal fraction) as follows:

$$(112)\ I_i = \sum_{j=1}^{n} I_{i,j}\left[\frac{kg_{lp}}{kg_{lp}\cdot d}\right] = \sum_{j=1}^{n}\left(\frac{Cn_i\left[\frac{kcal}{kg_{lp}\cdot d}\right]\times f_{diet\,i,j}}{\lambda_j\left[\frac{kcal}{kg_{lp}}\right]\times AE_j}\right)$$

where:

$I_{i,j}$	=	mass ingestion rate of dietary item *j* by organism *i* (i.e., kg_{lp} food/kg_{lp} body weight/day)
Cn_i	=	caloric ingestion rate of organism *i*
$f_{\text{diet } i,j}$	=	fraction of dietary item *j* in *i* diet
λ_j	=	caloric density of dietary item *j*
n	=	number of dietary items in *i* diet
j	=	specific dietary item *j*
AE_j	=	assimilation efficiency or fraction metabolizable calories of dietary item *j*

Using the flounder diet as an example, 2% is bottom sediments, 20% is polychaete, 20% is nematode, and 58% is lobster. Furthermore, using the caloric densities derived from Table 7 data, the caloric density of sediments as calculated above, the assimilation efficiencies (Fraction Metabolizable Energy from Gross) given in Table 7, and the flounder caloric ingestion rate of 82.9 $\frac{kcal}{kg_{lp} \cdot d}$ from Equation 110; we calculate the flounder ingestion rates as follows:

$$(113)\quad I_{fl,oc} = \frac{\frac{82.9\ kcal}{kg_{lp} \cdot d} \times 0.02}{\frac{11{,}456\ kcal}{kg_{oc}} \times 0.60} = \frac{0.000241\ kg_{oc}}{kg_{lp} \cdot d} \qquad I_{fl,nt} = \frac{\frac{82.9\ kcal}{kg_{lp} \cdot d} \times 0.20}{\frac{76{,}923\ kcal}{kg_{lp}} \times 0.65} = \frac{0.000332\ kg_{lp}}{kg_{lp} \cdot d}$$

$$I_{fl,pc} = \frac{\frac{82.9\ kcal}{kg_{lp} \cdot d} \times 0.20}{\frac{76{,}923\ kcal}{kg_{oc}} \times 0.65} = \frac{0.000332\ kg_{lp}}{kg_{lp} \cdot d} \qquad I_{fl,lb} = \frac{\frac{82.9\ kcal}{kg_{lp} \cdot d} \times 0.58}{\frac{29{,}412\ kcal}{kg_{lp}} \times 0.65} = \frac{0.000252\ kg_{lp}}{kg_{lp} \cdot d}$$

2.7.2.3 Assimilation Efficiencies Across Gastrointestinal Tracts

The assimilation efficiency (α) used in the governing equation (Equation 95) is specific to the chemical being assimilated and is not necessarily directly related to the assimilation efficiency of foodstuffs[34] (e.g., see Gobas et al., 1988; Endicott et al., 1991; Connolly, 1991; and Fisk et al., 1998). All of these aforementioned authors and others have attempted to develop a relationship between a chemical octanol-to-water partition coefficient (K_{ow}) and the assimilation of the chemical across the gastrointestinal tract. Based on data collected by Gobas et al. (1988) for various hydrophobic organic compounds, the following non-linear regression was developed (Gobas et. al, 1988; Equation 2):

$$(114)\quad 1/\alpha = 5.3 \times 10^{-8} K_{ow} + 2.3$$

where:

α = assimilation efficiency across gastro-intestinal tract (fraction)

K_{ow} = octanol-to-water partition coefficient [Liters/kg]

Endicott et al. (1991, Equations 38a, 38b, and 38c) found the following relationships based on a review of the available data collected from the scientific literature, again hydrophobic

[34] Matrix effects associated with the assimilation of chemicals have been identified, but the process of actually crossing the gastrointestinal tract is believed to be most associated with lipidophilicity (see Spacie and Hamelink, 1995; Kleinow and Goodrich, 1992).

organic compounds. Where the chemical $\log_{10}K_{ow}$ was below 6, α was equal to 0.90. For $\log_{10}K_{ow}$'s between 6 and 6.6 the following relationship was described:

$$(115)\ \alpha = 37.9 - 11.216 \log_{10} K_{ow} + 0.8409 (\log_{10} K_{ow})^2$$

For chemicals with a $\log_{10}K_{ow}$ greater than 6.6, Endicott et al. (1991) found that α was equal to 0.50. The degree of fit of the data and the relationships described by Endicott et al. (1991) is graphically presented but not extensively discussed in the manuscript. It is notable that no chemicals with a $\log_{10}K_{ow}$ below 4 appear to have been evaluated by Endicott et al. Further, the fit associated with chemicals with a $\log_{10}K_{ow}$ greater than 7 are very poor.

Fisk et al. (1998) similarly attempted to fit the relationship between K_{ow} and growth-adjusted α through regression analysis. These investigators recognized that assimilation efficiency data collected from the scientific literature might be affected by variable experimental designs, especially in consideration of foodstuff types, feeding rates, and complications associated with potential water exposures in addition to exposure through the food. These investigators used data collected from their experimentation only to develop a regression between K_{ow} and dietary assimilation. The form of the regression developed was parabolic with the form:

$$(116)\ \log_{10} \alpha = -1.8 + \log_{10} Kow - (0.08 \log_{10} Kow^2)$$

This regression was statistically significant (p=0.004), but the explained variation was low (r^2 = 0.53 where only 53% of the variation of α is explained by the regression).

It is clear that the methods and results described above are very different. It is notable that the efficiencies reported by Fisk et al. (1998) were specific to dietary exposures only, while many of the studies used by Endicott et al. (1991) relied on field observations. Figure 9 presents these estimation regressions across a range of K_{ow}s. The significant difference that lies within the $\log_{10}K_{ow}$ range from 5 to 7 is particularly troublesome. This range encompasses the majority of the bioaccumulative PCBs at issue within the PRAM.

Review of the raw data suggested that the form of the relationship between K_{ow} and α is perhaps best described as a parabolic function. A parabolic function was calibrated to assure a level of conservatism within the PRAM such that virtually all of the reported assimilation efficiencies fell below the predicted values. The resultant algorithm is presented below and graphically compared to the observed values reported by Gobas et al. (1988), Thomann (1989), and Fisk et al. (1998) in Figure 9.

$$(117)\ \alpha = \frac{10^{-1.8+1.08\log Kow - 0.08\log Kow^2}}{100}$$

2.7.2.4 Uptake Rate Constants and Assimilation Efficiencies Across Respiratory Tissues

The uptake rate (Ku_i) of a PCB can be calculated based on the respiration of the organism (r') and the relative assimilation efficiency between a chemical and oxygen (E) across respiratory tissue (e.g., see Thomann, 1989; Connolly, 1991):

$$(118)\ Ku_i\left[\frac{L}{kg_{lp}\cdot d}\right] = E \times \frac{r_i'\left[\frac{gO_2}{kg_{lp}\cdot d}\right]}{C_{O_2}\left[\frac{gO_2}{L}\right]}$$

where:

Ku_i = uptake rate constant for water in organism *i*

E = ratio between the assimilation efficiency for a chemical across respiratory tissue over the assimilation efficiency for oxygen across respiratory tissue (dimensionless)

r_i' = oxygen consumption rate

C_{O2} = dissolved oxygen concentration in water

The ratio between the assimilation efficiency for oxygen and that for a chemical has been related to the octanol-water partition coefficient (K_{ow}) of the chemical (Thomann, 1989, Equation 22), such that E can be derived from the chemical $\log_{10}K_{ow}$ and the body weight (wet weight) range of the organism(s). For chemicals with a $\log_{10}K_{ow}$ between 2 and 5 and organisms weighing less than 100 grams, E can be calculated using the following relationship (Thomann, 1989):

$$(119)\ \log_{10} E = -2.6 + 0.5\log_{10} Kow$$

Where the $\log_{10}K_{ow}$ is between 5 and 6 and the organism is less than 100 grams in body weight, E is equal to 0.80. Where the $\log_{10}K_{ow}$ is between 6 and 10, E can be calculated as follows:

$$(120)\ \log_{10} E = 2.9 - 0.5\log_{10} Kow$$

A different set of relationships between $\log_{10}K_{ow}$ and E apply for organisms greater than 100 grams in body weight (Thomann, 1989). Where $\log_{10}K_{ow}$ is between 2 and 3:

$$(121)\ \log_{10} E = -1.5 + 0.4\log_{10} Kow$$

Where the $\log_{10}K_{ow}$ is between 3 and 6, E is equal to 0.50, and where the $\log_{10}K_{ow}$ is between 6 and 10:

$$(122)\ \log_{10} E = -1.2 + 0.25\log_{10} Kow$$

This approach to estimate the efficiency of the transfers of PCBs across respiratory tissues for invertebrates, however, is not the most accurate and theoretically appropriate for fish (Barber, 2003). Barber (2003) suggests a correction to the uptake rate that is appropriate for fish and has been incorporated into the PRAM:

$$(123)\quad Ku_{fish-i}\left[\frac{\mathrm{cm}^3}{\mathrm{g_{ww}}\cdot d}\right] = 0.343\times\left(\frac{1400\mathrm{W}[\mathrm{g-ww}]^{-0.4}\mathrm{K_{ow}}}{100+\mathrm{K_{ow}}}\right)^{1.048}$$

where:

Ku_{fish-i}	=	uptake rate constant for water in fish *i*
W	=	fish body weight in grams wet weight (ww)

Unit conversions of Barber's uptake rate are accomplished in PRAM as follows:

$$(124)\quad \mathrm{Ku}_{fish-i}\left[\frac{\mathrm{L}}{\mathrm{kg}_{\mathrm{lp}}\cdot \mathrm{d}}\right]=\mathrm{Ku}_{fish-i}\left[\frac{\mathrm{cm}^3}{\mathrm{g}_{ww}\cdot \mathrm{d}}\right]\times\left(\frac{1}{\left(1-\mathrm{f}_{moist,i}\right)}\frac{\mathrm{g}_{\mathrm{ww}}}{\mathrm{g}_{\mathrm{dw}}}\right)\times\left(\frac{1}{\mathrm{f}_{lp,i}}\frac{\mathrm{g}_{\mathrm{dw}}}{\mathrm{g}_{lp}}\right)\times\left(\frac{1000\ g_{lp}}{kg_{lp}}\right)\times\left(\frac{1\ L}{1000\ cm^3}\right)$$

2.7.2.5 Depuration Rates (Elimination and Metabolism)

Depuration is the sum of the loss due to metabolism and/or excretion of the PCB. When assuming no growth, the lipid-based elimination rate (Ke_i) can be related to the K_{ow} (Thomann, 1989; also Connolly, 1991) and the uptake rate constant such that:

$$(125)\ Ke_i\left[\frac{kg_{PCB}}{kg_{lp}\cdot d}\right]=\frac{Ku_i}{Kow}$$

This excretion rate does not account for any metabolism of the chemical by the animal. For certain PCBs (e.g., the heavy PCB series such as hepta-CB, octa-CB, etc.), such an assumption is valid, but for less chlorinated forms (e.g., mono-CBs, di-CBS, and tri-CBs), this assumption is not valid. To account for at least a minimal metabolism of the PCBs, the following K_{ow} – elimination (Ke) regression based on larval saltwater fish was evaluated (obtained from Petersen and Kristensen, 1998, Table 4):

$$(126)\ \log_{10} Ke\left[\frac{1}{day}\right]=3.25-0.66\times\log_{10} Kow$$

This can be considered a conservative approach as the metabolic activities of larval fish is quite limited (Peterson and Kristensen, 1998) and the modeled metabolism would be underestimated for many of the more juvenile and adult forms.

A similar approach was taken where additional elimination rate constants, as obtained from the literature, were evaluated in the context of the algorithm obtained from Peterson and Kristensen (1998) to assure that the algorithm produces conservative estimates. A new regression of elimination rates (Figure 10) reported by Peterson and Kristensen (1998), Thomann (1989) and Fisk et al. (1998) result in slightly lower predicted Ke than that of Petersen and Kristensen (1998):

$$(127)\ \log_{10} Ke\left[\frac{1}{day}\right] = 1.065 - 0.4131 \times \log_{10} Kow$$

In spite of the metabolism that occurs in many species for the less chlorinated PCBs, the most conservative approach to modeling bioaccumulation in PRAM is to ignore such metabolism in all species. Gobas and Mackay (1987) developed estimates of several bioenergetic parameters by analyzing data from several other researchers. For the estimation of elimination rates, exclusive of metabolism, Gobas and Mackay derived the following relationship between K_{ow} and Ke_i:

$$(128)\ \frac{1}{Ke_i\left[\dfrac{kg_{PCB}}{kg_{lp}\cdot d}\right]} = 0.00089Kow + 0.075$$

Gobas and Mackay compared this equation to experimental data obtained by other researchers for PCBs in fish and found that it fit the data well. Although it does not include any metabolism of the PCBs, equation 128 has been used in PRAM to estimate depuration rates.

2.7.2.6 Derivation of Growth Rates from Bioenergetic Budget

To estimate the temperature-related growth rate of an organism (G), the bioenergetic budgets of the organism are once again used. The growth rate (G) is calculated from the relationship between Cn and G (assuming G includes reproduction – see Welch, 1968) and the caloric density (λ) of the organism:

$$(129)\ G_i\left[\frac{\mathrm{kg_{lp}}}{\mathrm{kg_{lp}}\cdot \mathrm{d}}\right] = \frac{\left(Cn_i\left[\dfrac{kcal}{kg_{lp}\cdot d}\right]\times f_{grow,i}\right)}{\lambda_i\left[\dfrac{kcal}{kg_{lp}}\right]}$$

To reiterate the energy budget for flounder, 20% is used for production (growth and reproduction – Table 7). Thus, the flounder growth rate, for example, is calculated as follows:

$$(130)\ G = \frac{\frac{82.9\ kcal}{kg_{lp} \cdot d} \times 0.20}{\frac{22{,}272\ kcal}{kg_{lp}}} = 7.44 \times 10^{-4}\ \text{day}^{-1}$$

Input parameters required for the PRAM include environmental conditions associated with the site where the vessel will be sunk, the vessel dimensions, and the character and amount of PCB-containing materials onboard the vessel. This information is presented in this section, using the ex-ORISKANY as an example. Future evaluations using PRAM must use site-specific information for the vessels and their site environmental conditions. The impact of variability of input parameters on the model output is addressed under the Uncertainty section in Section 4.

3.1 PHYSICAL BOUNDARY AND CONDITIONS

The ex-ORISKANY (CVA-34) has a displacement of 27,100 tons, a length of 888 feet, a hull width of 93 feet, and an extreme width of 147.5 feet, or an average beam of 120 feet. The depth of the water at the proposed site of sinking of the vessel is 212 feet, and if the vessel is correctly sunk, it should stand about 150 feet off the sea floor, with a maximum potential height of 157 (if set on the sea floor at a 90° angle) (FWCC, 2004). It is anticipated that the vessel will sink some feet into the sand bottom sea floor (FWCC, 2004).

The sea floor substrate in the vicinity of the site is characterized as fine sandy unconsolidated deltaic sediments underlain by limestone (NAVSEA, 2004). Sediment thickness varies from little to none (limestone outcroppings) to several feet (NAVSEA, 2004). Typical organic carbon content in deep water sediments such as those associated with the Large Area Artificial Reef Site (LAARS) is reported to generally be 1% or less (Parsons et al., 1977). The "bio-active" zone within a sediment bed is generally about 10 cm in depth, where the vast majority of organisms, aside from unicellular bacteria and fungi, reside and feed (e.g., see Bosworth and Thibodeaux, 1990). This depth into the sediment bed also represents the "bioturbation" zone, where the sediments within this layer are well mixed due to the physical movement of the organisms present (Bosworth and Thibodeaux, 1990). The bioactive sediment depth represents not only an exposure media for PCBs but also a potential sink or sequestering media. While the sediment contributes to the entry of PCBs into the benthic food chain, it also directly competes as a sorption site, sequestering PCBs away from the pelagic and reef food chains. Thus the larger the sediment bed the greater the sequestering of PCBs.

Water quality at the proposed ex-ORISKANY Memorial Reef site is suggested to be "pristine" with high dissolved oxygen levels, approaching saturation (NAVSEA, 2004). The yearly average (year 2001) surface water temperature at the nearby NOAA (National Oceanic and Atmospheric Administration) data buoy #42040 was 24.5°C with a minimum temperature of 16.7°C and reported maximum of 32.4°C (NOAA NDBC, 2004, (http://www.ndbc.noaa.gov/station_history.phtml?station=42040). Averaging all of the daily temperature data for buoy #42040 from 2002 to 2004 also resulted in a sea surface water temperature of 24.5°C. Given this water temperature and assuming that the dissolved oxygen (DO) is near saturation (90% of saturation) for most of the year, a dissolved oxygen concentration can be calculated, 6.12 mg/L.

As discussed previously, the PRAM comprises four distinct water compartments: the outside surface of the vessel, below the pycnocline,[35] the water above the pycnocline, the water within the interior spaces of the sunken vessel, and the interstitial or pore water within the sediment bed. The average water temperature for the water compartment above the pycnocline is assumed to equal the average sea surface water temperature, 24.5°C. The average water temperature for the water compartment below the pycnocline was estimated by averaging data from the Mississippi-Alabama Marine Ecosystem Study (MAMES) Mooring B buoy, which measured temperatures at a depth of 187 feet from December 1987 to October 1989 (USGS and MMS, 1999, *Ecology of Live Bottom Habitats of the Northeastern Gulf of Mexico: A Community Profile*). The average water temperature for a depth of 187 feet was 19.5°C, with a range of 17°C to 22°C. The average temperature for the water below the pycnocline, 19.5°C, is also assumed to be the average water temperature within the interior spaces of the sunken vessel and the interstitial water within the sediment bed. Within the sunken vessel and sediment bed, it is assumed that the water is more stagnant and thus would be expected to contain less dissolved oxygen. Thus, the vessel interior DO concentration is assumed to be 75% of the vessel exterior DO concentration, while the sediment pore water is assumed to be 50% of the surface water DO.

Total suspended solid (TSS) concentrations in the ocean are highly variable and care must be taken in using values that include phytoplankton, as the phytoplankton are considered as a separate compartment within the PRAM. A value of 10 mg/L is the default value for total suspended solids within the PRAM based on the general oceanographic literature (e.g., Parsons et al., 1977). Similarly there is little information regarding the "typical" organic carbon content levels for suspended solids. Parsons et al. (1977) report that between 16% and 52% of the true detritus (non-living particles) is degradable by bacteria; given this, a conservation assumption that the organic carbon content is 15% was made.

[35] The pycnocline is assumed to form at 15 meters of depth and is considered a continuous boundary within the PRAM.

Dissolved organic carbon concentrations in near surface waters (less than 100 meters), range from 0.6 to 2.0 mg/L (Parsons et al., 1977). No site-specific information is available for the ex-ORISKANY Memorial Reef site therefore the PRAM default value of 0.6 mg/L is assumed to be functional here.

Wind-driven water currents are low in the vicinity of the expected sinking site and are reported to be generally less than 0.5 knots or 0.58 mph (FWCC, 2004). These currents are also expected to dissipate with depth. Horizontal up-currents have been reported for the area but are not included within the PRAM. Two currents are used in the PRAM to calculate advective transport of any PCBs released from materials within a sunken vessel: the prevailing current outside the vessel and the current within the vessel transporting any released PCBs to the exterior of the ship. Current and eddies within the vessel are surely variable and not unidirectional. Nevertheless, within the PRAM, the interior current is used to calculate the flux of PCBs to the exterior of the vessel. The outside current will cause movement of water within the vessel and as such, the interior is set as a dependent variable (fraction) of the prevailing water current; 1% of the outside current velocity (0.0058 mph).

Many of the less chlorinated PCBs (e.g., mono and dichlorobiphenyls) will volatize from the water into the air such that this is a loss term for the model. The PRAM incorporates an air compartment directly above the modeled oval cylinder of the ocean and the artificial reef. The default height for this compartment is 10 meters. It is unlikely that any volatilized PCBs would attain a height greater than this before being transported out the modeled system via wind current. The overall average wind current for the area associated with the ex-ORISKANY Memorial Reef site is reported to be 7.4 knots or 8.5 mph (FWCC, 2004).

The environmental parameters used for evaluating the ex-ORISKANY are presented in Table 9.

3.2 PCB MASS LOADING WITHIN THE PRAM SUNKEN VESSEL (EX-ORISKANY) MODEL COMPARTMENT

The ex-ORISKANY has been prepared for use as an artificial reef. The preparation included removal and/or reduction of PCB-containing materials. Following preparation, six bulk product materials containing PCBs remain onboard: bulkhead insulation (BHI), foam rubber, rubber pipe hanger/liner materials, paints, electric cable insulation, and ventilation gaskets (inner and outer gasket material). The PCB concentrations in these materials onboard the ex-ORISKANY have been reported by Pape (2004) of CACI (Fairfax, Virginia) for NAVSEA.

These data were compiled and subjected to statistical analysis. The appropriate concentrations to be used in the PRAM, based on general risk assessment guidance are the 95% upper confidence limits for the mean. The 95% upper confidence limits are statistically derived according to the logic diagram presented in Figure 11. The results of the statistical analysis are summarized in Table 10 and detailed in Appendix A.

What is notable in the data collected from the PCB-containing materials is the degree of variability of the PCB concentrations within each material. This variability is illustrated with Box-Whisker diagrams in Figure 12. The top plot for each material is on a linear scale whereas the lower plot is on a log scale. The most extreme case of variable PCB concentrations occurs in electrical cable and bulkhead insulation materials. There are strong indications of statistical outliers for these data sets. However, removal of some of the outliers did not normalize the PCB concentrations found in bulkhead insulation material, for example (see Appendix A). While some of the sampling data are highly variable, the use of the 95% upper-confidence limits for the mean produced a “worst-case” condition and are, as such, suitable for assessing the potential risks associated with these materials.

The concentrations of the PCBs within these materials are, by themselves, insufficient to estimate the potential risks associated with the vessel. The mass of the PCB-containing materials is also required to estimate the total mass of PCBs available for leaching in order to evaluate the potential risk and and/or hazard to people consuming marine organisms collected from the prospective reef. Estimates of the total mass of PCB-containing materials have been made from data included in *Final Polychlorinated biphenyls (PCB) Source Term Estimates for ex-ORISKANY report, revision 4* (CACI, 2004). In this report, CACI began the derivation of the source term mass estimates by referencing a Final Weight Report (FWR) for the USS Essex; then assumed that the USS Oriskany had the same amount of mass as the USS Essex for each source term. It should be noted that although there is an uncertainty associated with this method, the USS Essex (CVA-9) and USS Oriskany (CVA-34) belong to the same vessel combatant class (Essex), and were constructed around the same time period.

Table 13 of the CACI report contains the initial source-term masses (in units of pounds of PCB containing materials), the growth of the masses over the 30-year life of the ship and the present reduction for each material that was achieved during removal actions. To estimate the mass of the source terms present on the ex-ORISKANY after cleanup actions were completed, three adjustment factors were applied to the FWR masses presented in the CACI report.

The first adjustment factor corrects for a discrepancy between the electrical cable source term used in PRAM and the source term estimated in the CACI report. For electrical cable, the CACI report estimated the mass of cable insulation while PRAM utilizes a mass value for intact electrical cable (wires plus insulation). The CACI report estimates that the cable insulation represents 72.26% of a typical intact cable, therefore an adjustment factor of 1.384 (i.e., 1/0.7226) is required to account for the additional mass of the wires in the PRAM source term.

The second adjustment factor accounts for the growth of initial source term quantities over the life of a ship. Items such as paint are reapplied frequently and therefore increase dramatically over the life of a ship, while other materials are untouched or replaced with an equivalent mass of the same material and therefore do not change at all. Growth factors were developed for various bulk materials to account for reapplication. The growth factors used are the same as those specified in the CACI report.

The third adjustment factor accounts for the removal of materials during the preparation of the ex-ORISKANY for sinking. Materials such as lubricants were completely removed prior to sinking, while others are not removed at all. A significant amount (72.6%) of bulkhead insulation material was removed during preparation activities. The adjustment factors used in PRAM are the ones reported by CACI in the December 2004 report. No further removal actions are anticipated, but if additional materials are subsequently removed the default ex-ORISKANY adjustment factors will need to be revised.

The mass values entered into PRAM represent the FWR masses multiplied by each of the three adjustment factors. The original FWR masses, the three adjustment factors, and the current masses entered into PRAM are tabulated in Table 11 with units of both pounds and kilograms (PRAM accepts units of kilograms). The source-term mass values shown in this table are consistent with the mass estimates used in the TDM modeling effort (see Time Dynamic Model [TDM] Documentation).

3.3 THE ZONE OF INFLUENCE FOR THE EX-ORISKANY MEMORIAL REEF

One significant outstanding question regarding PRAM for use in the Navy artificial reef program (REEFEX) is development of a “zone of influence” (ZOI) to provide multidimensional spatial boundaries for exposure estimation. Consultations with USEPA and State of Florida through the TWG led the Navy to finalize the ZOI concept. As such, it is an “exposure volume,” consisting of a column of water with an oval-shaped footprint extending from the seafloor to the surface.[36] The lateral dimension of the column is derived via a factor multiplied by the volume of the ex-ORISKANY (which is roughly 54,000 cubic meters). That is, at a multiplier of one (1) the lateral extent of the ZOI is essentially zero and the exposure volume becomes that of the column extending between the upper surface of the vessel to the water/air interface (i.e., the volume of the vessel subtracted from the total volume of the column).

Using a multiplier of two (2), the "diameter" of the column (length and width of the oval) is increased by about 30 meters, producing a horizontal aqueous space of about 15 meters from the vertical edges of the vessel. This allows for a common space for exposure to benthic invertebrates, demersal fish, and nektonic animals occupying the water surrounding the vessel (both laterally and above) and occupying the sediment surrounding the vessel (see Figure 11). Based on consensus reached by the TWG, the column is divided by a pycnocline which is a horizontal boundary dividing the upper and lower masses of water due to differences in salinity and temperature (see Section 2.2.2).

3.3.1 Habitat and Dietary Composition as Factors for Determining ZOI

The Navy acknowledged in the draft Supplemental Human Health Risk Assessment (SHHRA) for the ex-ORISKANY (NEHC, July 2004) that the ZOI multiplier value of 5 was subjective, as the value was not backed up by documented technical basis such as statistical information concerning the degree of change in PCB concentrations as a function of increasing ZOI multiplier value. Subsequent to the draft SHHRA and upon consultations with USEPA and State of Florida in the TWG, the Navy determined that the documented technical basis should be based on potential exposure (possible presence of receptors with the assumption that environmental media surrounding the sunken vessel would contain PCBs) rather than concentration gradient. As a result, the Navy prepared a paper that presented summary information regarding biological factors related to potential PCB biouptake that should be considered in choosing an appropriate ZOI multiplier value(s). Based on the paper (NEHC, 2005), ZOI recommendations for the ex-ORISKANY were presented. Additional information describing the composition of fish assemblies that might be associated with the artificial reef ex-ORISKANY, and information of relevance to establishing spatial boundaries for those assemblies, are presented in Appendix F.

[36] There was agreement between the EPA and the Navy in the Nov 17-18, 2004 TWG meeting that the water column above the seafloor should be divided into two regions, i.e., water above and below the thermocline (pycnocline) with the pycnocline occurring approximately 55 feet below the sea water surface.

3.3.1.1 Verticality

Among the many factors perceived to influence the composition and local distribution of fish assemblages associated with both natural and artificial structures in marine environments, “verticality” is clearly significant (e.g., many of the listed references based on studies by D.R. Stanley and C.A. Wilson [and others cited therein]). The verticality issue is comparatively straightforward, as it must include the entire water column height. Many types of fish reside throughout the height of the water column; others would use various layers throughout the column. Most of the plankton-feeding fishes (e.g., vermilion snapper) tend to feed on the upper zone of the water column. The same is true for most of the pelagic predators in pursuit of schooling forage fishes (e.g., anchovies and herring; Bortone, 2004). The upper zone is also important for production of the phytoplankton that “rain down” to lower layers to provide a significant fraction of the energy for their inhabitants. Inclusion of space for habitats (and their biotic occupants) lateral to the vessel must also be considered.

The aforementioned and many other studies, such as one compilation focusing on natural hard bottom habitats in the general vicinity of the proposed ex-ORISKANY site (Thompson et al., 1999), indicate substantial variability in biotic community composition with both sea depth and “shape” of submerged structures.

Considering the available relevant literature and the extraordinarily unusual size and shape of ex-ORISKANY, the Navy deemed that it was nearly impossible to predict community composition and/or structure in much detail, albeit abundances and availability of certain food fish in relation to each other are more predictable.[37] For purposes of PRAM, however, the uncertainty of detailed taxonomic composition is moot. The habitats provided by the vessel will almost certainly be exploited by a wide range of transient and (at least effectively) resident fishes. Some of the latter will tend to be associated with relatively short depth ranges in the context of the immense height of the vessel, including areas lateral to the hull (i.e., in its “shadow” for purposes of this discussion).

The shadow-dwellers (resident fishes that tend to be associated with areas lateral to the hull for short distances) will be a mixture of fishes that tend to feed on encrusting organisms and

[37] Per personal communication with Jon Dodrill, Florida FWCC (01-05-05), food fishes listed in Attachment 1 (GMFMC [2003] table), that are most likely to be more abundant than others at the ex-ORISKANY are: red snapper, vermilion snapper, gag, scamp, gray snapper, gray triggerfish, greater amberjack, almaco jack, red grouper. Others may be present at some time or another but are much less common (i.e., Warsaw, black grouper, speckled hind, goliath grouper [protected], etc.) while some, like yellowtail snapper, may be outside their normal geographic range in this area.

thus are tightly associated with the structure per se (e.g., gray triggerfish; Beaver, 2004), as well others that tend to forage on or near the seafloor adjacent to the structure (e.g., red snapper; Gallaway et al., 1999; Ouzts and Szedlmayer, 2003). For example, there are several studies suggesting that such fishes can have substantial impact on the benthic communities adjacent to both natural and artificial submerged structures (e.g., Frazer and Lindberg, 1994; Lindquist et al., 1994; Steimle and Figley, 1996; Nelson and Bortone, 1996; Bortone et al., 1998).

3.3.1.2 Horizontal Extent

To determine the lateral extent, specifically, the minimum lateral aqueous space that would satisfy the needs of the shadow-dwellers, the Navy (NEHC 2005) was attempting to find the lateral extent or distance necessary to capture a large fraction of the foraging areas of various legitimately "reef-associated" fishes. However, it found that such a distance is essentially un-documented for the vast majority of reef fish.

In reviewing representative samples of relevant literature, there are two general types of studies that provide evidence for at least an order of magnitude for the foraging distance. These types are: (1) density estimates based on surveys, especially those using dual-beam hydroacoustic technology (e.g., the series of studies reported by Stanley and/or Wilson); and (2) tagging studies, especially those related to movements among fragmented habitats (e.g., Bardach, 1958; Springer and McErlean, 1962; Low and Waltz, 1991; Chapman and Kramer, 2000).

The density-estimate data suggest that for various submerged structures there tend to be recognizable boundaries of fish aggregations in the range of 20 to 50 meters from the structures.[38] Most of the tagging studies tend to show that many of the more common species (hence the ones for which more data are available) seldom, if ever, move more than a few to several tens of meters, at least over the timeframe of the particular study. Note that, of course, there are tagging records that document movements of fishes on the scale of hundreds of kilometers, but most of these (e.g., sturgeon, salmon) are not related to species that are known or considered reef-associated (at least as adults).[39] Another consideration is a factor

[38] The distances of 20 and 50 meters approximately correspond to ZOIs of about 2.5 and 5, respectively, for the ex-ORISKANY.

[39] Per personal communication with Jon Dodrill, Florida FWCC (01-05-05), juveniles and subadults of reef associated species may be more prone to movement than older adults inhabiting at deeper offshore sites such as the ex-ORISKANY. The older adults (younger adults just over the legal limit, e.g., 3-6 year old red

mentioned in some of the Stanley and/or Wilson series of studies, which is the typical maximum range of vision in fish. This factor, among others, may influence how far fish tend to range from their shelter or habitat. This distance is about 15 meters in clear water (Gerking, 1994), and would obviously be smaller with increasing turbidity.

3.3.2 Discussion/Recommendations

Based on the foregoing, it seems reasonable to use a single exposure volume to minimize complexity. Thus, a ZOI multiplier between two and five for the ex-ORISKANY is recommended, if there is a consensus regarding degree of conservatism. Figure 13 presents the vessel dimensions and the relationship between lateral distance from the edge of the vessel and ZOI. For the ex-ORISKANY, doubling the ZOI (using a ZOI multiplier value of 2) would provide about 15 meters of lateral aqueous space from the vertical sides of the vessel, which would correspond to some of the lower estimates of "reef-fish" aggregation sizes (as well as the range of visibility of the "typical" fish). Quadrupling the ZOI (using a ZOI multiplier value of 4) would roughly double the lateral dimension (to ~40 meters from the vertical sides of the vessel), which would correspond roughly with some of the higher density discontinuity observations. Using a ZOI multiplier of 5 would correspond to a approximately 50 meters from the vertical sides of the vessel, which would capture the range indicated by studies using density estimates. Stated another way, a multiplier of 2 would likely "capture" at least some fraction of the foraging range of most of the "reef-fish" aggregation members, whereas a multiplier of 5 would likely capture most of the foraging ranges of most of the fishes.

Alternatively, one might consider multiple ZOIs, still based on the vessel volume, but accounting for various spatially limited groups of species (e.g., a ZOI based on a multiplier of 2 for encrustation-grazers such as the gray triggerfish, and ZOI of 4 to 5 for less reef-

snapper), although with higher site fidelity, are subject to intense fishing pressure such that few of the target food fishes will survive multiple years at the ex-ORISKANY site. The juveniles and subadults, and even young adults, are likely to make permanent non-return movements away from the reef, after weeks/months. Movement is also facilitated by major storm disturbances in the easterly or southeasterly direction. Hence, it is agreed that PRAM ZOI, as recommended, is highly conservative for the targeted food reef fish based on the assumption that they are going to spend their entire lives in an imaginary aquarium zone of influence in the immediate vicinity of the ship. The situation is different with strongly reef obligate species (e.g., damsel fishes such as cocoa damsels, cubbyus, tomtates, blennies, belted sandfish, etc.) that are not targeted as food fish. They may well spend an entire life from post larval to "old" age (barring predation or disease) on the ship or even one part of it. Exception would be gray triggerfish- they would be the one food fish probably exhibiting highest consistent site fidelity over a period of years if they survived harvest and natural predation.

associated fish, based on the evidence of fish fidelity around a submerged structure and a reasonable volume for PCB leaching and transport).

Based on professional judgment, biology, and modeling considerations, the recommendations for the ex-ORISKANY, are:

- ZOI for near-field foraging species, such as the gray triggerfish: 2 to 2.5
- ZOI for less reef-associated fish species, i.e., pelagic fishes and benthic fishes: 4 to 5

This section presents the methods used to assess risks and hazards based on input into the risk characterization module within PRAM. The approaches used to calculate abiotic modeling output (air, water, and sediment concentrations) and biotic modeling output (vertebrate and invertebrate tissue concentrations) were presented in Sections 2 and 3. The risk modeling output of PRAM provides estimates of cancer risks and non-cancer hazards to individuals eating these organisms on a long-term (chronic) basis. It should be noted that, because PRAM is a steady-state model, it does not calculate risks or hazards on a short-term (subchronic) exposure associated with the first two years after a ship is sunk when the reef-associated biological community is still developing.[40] In other words, the PRAM characterizes risks to humans from the two-year point and onward.

The methodology applied in PRAM is based on standard regulatory risk assessment procedures, as identified in the *Risk Assessment Guidance for Superfund, Volume 1, Human Health Evaluation Manual (Part A)* (RAGS) (USEPA, 1989). Per the technical approach identified in RAGS, human health risk assessment typically consists of four distinct components:

- Data Evaluation
- Exposure Assessment
- Toxicity Assessment
- Risk Characterization

A discussion of the assumptions and algorithms for each of these components, as implemented in PRAM's risk characterization module, is provided in the following sections. Figure 14 presents the risk characterization model and its relationship with other components of the process flow to estimate chronic risks.

4.1 CHEMICAL DATA EVALUATION

RAGS states that chemical data, in terms of the concentrations of chemical contaminants in an environmental medium, are needed to estimate the degree of exposure. As presented in

[40] The PRAM's food chain (food web bioaccumulation) and risk assessment algorithms can, however, be used in conjunction with another model's outputs (the Time Dynamic Model [TDM]) to estimate risks associated with subchronic ingestion of fish and shellfish during the first two years after the ship is sunk, as the reef community is still developing. For a description of how the TDM outputs are used in conjunction with PRAM's food chain and risk assessment algorithms to derive estimates of subchronic risks, see Time Dynamic Model (TDM) Documentation (NEHC/SSC-SD, May 2005).

the site conceptual exposure model (SCEM; Figure 15), the medium that is most likely to produce human exposure to PCBs is the tissue of potentially edible marine species at or in the vicinity of the sunken artificial reef. This concentration is known as the "exposure point concentration."

PRAM calculates site-specific, whole body tissue concentrations for all ten PCB homolog groups in representative reef sport fish and invertebrates, bottom dwelling (sediment associated or benthic) sport fish and invertebrates, and open-water (pelagic) sport fish within the ZOI of the artificial reef. As described in Sections 2 and 3, the predicted tissue concentrations are highly dependent on a number of site-specific variables, including PCB source concentrations, mass of PCB source material, physical properties of the reef and reef environment, ZOI, and chemical-specific values, such as the octanol-water partitioning coefficient (K_{ow}). For each representative species, the biotic-food web PRAM module sums the homolog concentrations to arrive at an estimated concentration of total PCBs. These whole body, total PCB tissue concentrations serve as exposure point concentration "inputs" into the risk characterization module, where they are used to calculate chronic risks and hazards. Because different organisms bioaccumulate PCBs differently from one another, and because anglers may preferentially target different species of sports fish, PRAM calculates tissue concentrations in representative species from the following biological compartments/groups:

- Benthic Fish (Trophic Level [TL] IV Benthic Predator)
- Benthic Invertebrates (TL III Benthic Invertebrate Foraging Predator)
- Pelagic Fish (TL IV Pelagic Predator)
- Reef Fish (TL IV Reef Predator)
- Reef Fish (TL III Reef Vertebrate Forager)
- Reef Invertebrate (TL III Reef Invertebrate Forager)

These groups were chosen as containing targeted sports fish (both finfish and shellfish), as well as representing the groups with greatest potential for PCB biouptake/bioaccumulation. Exposure point concentrations derived for each group will vary from one reef site to another, based on variations in depth, temperature, local species, fishing preferences of local angler populations, etc., and therefore should be evaluated on a site-specific basis.

4.2 EXPOSURE ASSESSMENT

RAGS states that an exposure assessment must be conducted to identify the source of contamination, release/transport, receptor, and route of exposure before a risk assessment can be conducted. When all these elements are present, one can then conclude that the "exposure pathway" is complete. Without a complete exposure pathway, there will be no risks, as exposure does not occur.

The SCEM identifies a potentially complete exposure pathway represented by the release of PCBs from residual bulk products (source) by leaching, subsequent transport and distribution of released PCBs in the environment, including organisms (biota) at the sunken artificial reef, and ingestion of these organisms by recreational anglers. This scenario was chosen for evaluation, as it represents a reasonable worst-case scenario, addressing potential risks to local populations who would be expected to visit the reef on a regular basis, and who eat the fish they catch. In addition, because fish caught at the reef could be brought home and eaten by children (i.e., a more sensitive population than adults), ingestion of fish by children has been included in PRAM as a conservative (i.e., health-protective) measure.

With exposure parameters, such as frequency and duration, and fraction of fish ingested, the exposure point concentration, the risk characterization module in PRAM quantifies exposure in terms of "intake" by calculating the amount of PCBs that the receptors (anglers and their children) are likely to consume from the contaminated fish. Intake is expressed in mass of PCBs ingested per unit mass of body weight per day. The intakes used in the calculation of risk are based on combined child and adult exposure, as well as for children only.

Intakes are estimated in PRAM following USEPA-recommended approaches to derive both Reasonable Maximum Exposure (RME) and Central Tendency Exposure (CTE). The RME calculations use a number of upperbound exposure assumptions to provide a reasonable estimate of upperbound exposure among angler populations. The CTE calculations are based on a number of mid-range exposure assumptions, and are intended to represent risks and hazards to the typical angler.

Most of the exposure parameters used to quantify exposure to anglers and children are standard USEPA default values that are judged to be applicable to any reef site, with two exceptions: Fraction of Fish Ingested (FI) and Fish Ingestion Rate (IR). These two parameters are site-specific input values that must be identified for the risk characterization module in PRAM. For the ex-ORISKANY artificial reef site, an FI term was derived based on a Fish Consumption Survey conducted by the Escambia County Marine Resources Division (ECMRD, 2004). The FI value defines the relative proportion of fish an angler (or a child) eats from the reef relative to the total amount of fish in his or her diet from all sources (caught in other fishing areas, purchased at stores, etc.). In the absence of site-specific information, the FI value in PRAM can be set as 1.0 (i.e., a highly conservative assumption that the reef is the only source of fish in a person's diet). The IR value reflects variation in the amount of fish various populations consume in different regions of the United States. USEPA-recommended, region-specific fish ingestion rates, as reported by the National Marine Fisheries Service (NMFS, 1993), can be found in Table 10-52 of the *Exposure Factors Handbook* (USEPA, 1997). For the ex-ORISKANY site evaluation, the IR value for the Gulf States is used. Other exposure parameters used in the ex-ORISKANY risk evaluation are presented in the risk equations in the Risk Characterization section (Section 4.4).

4.3 TOXICITY ASSESSMENT

In addition to exposure assessment, RAGS requires that a toxicity assessment be conducted. Toxicity assessment defines the inherent "toxic" nature of the chemical contaminant. The toxic characteristic of the chemical is represented by its ability to elicit cancer and non-cancer effects (adverse, systemic effects on the body) from the exposure, and is measured in terms of dose and response (likelihood or degree of injury/effect per unit exposure). The USEPA's Office of Research and Development conducts toxicity assessments of chemicals used in health risk assessment; commercial mixtures of PCBs (not those found in the environment) are among the chemicals evaluated. Toxicity values for total PCBs (reference doses [RfDs] and slope factors [SFs]) used in PRAM were obtained from USEPA's Integrated Risk Information System (IRIS) database located at URL:

http://www.epa.gov/iriswebp/iris/index.html

The RfD is defined by USEPA as an estimate (with uncertainty spanning perhaps an order of magnitude) of a daily exposure to the human population (including sensitive subgroups) that is likely to be without appreciable risk of deleterious [non-carcinogenic] effects. The SF is an upperbound estimate of the incremental cancer risk for humans and is expressed as the probability of risk per milligram (mg) of chemical exposed per kilogram (kg) body weight per day for lifetime exposure. The SFs are derived mathematically by USEPA using extrapolation models with animal or human data, and the resulting SFs are highly conservative slopes or rate constants that correspond to the 95th percentile confidence level to predict excess cancer occurrence per life time.

IRIS provides RfD values for two total PCB mixtures, Aroclor 1254 (RfD of 7x10^{-5} mg/kg-day) and Aroclor 1016 (RfD of 2x10^{-5} mg/kg-day). Of these two values, PRAM uses the more conservative (health-protective) RfD of 2x10^{-5} mg/kg-day, based on Aroclor 1254, for RME scenario. A RfD of 4.5x10^{-5} mg/kg-day, which is the arithmetic mean of the Aroclor 1016 and 1254 RfDs, is used for CTE scenario. This value was chosen based on the assumption that aroclors at the ship are likely to represent a mixture of PCBs.

IRIS recommends two different slope factors for evaluating cancer risks from ingestion of total PCBs from the food chain. A slope factor of 2.0 (mg/kg-day)$^{-1}$ is recommended for RME calculations, and a slope factor of 1.0 (mg/kg-day)$^{-1}$ is recommended for CTE calculations.

These RfD and SF values are assumed to be applicable to both adults and children in PRAM.

4.4 RISK CHARACTERIZATION

According to RAGS, risk is a combination of toxicity and exposure. Based on intake and toxicity of PCBs, the risk characterization module in PRAM calculates potential cancer risks and non-cancer hazards to recreational angler populations (and their children) who consume fish caught at a reef on a long-term basis.

Risk calculations (risk characterization) are performed using standard USEPA equations as presented in RAGS. Non-cancer hazard, based on child exposure only, is calculated using equation 131. Hazard based on combined adult and child exposure is presented in equation 132.

$$(131)\quad HI_c = \frac{(C_f * IR_c * FI * EF * ED_c)}{(BW_c * AT_{nc\_child})} * \frac{1}{RfD}$$

$$(132)\quad HI_{a\&c} = \frac{(C_f * FI * EF * \left(\frac{IR_c * ED_c}{BW_c} + \frac{IR_a * ED_a}{BW_a}\right)}{AT_{nc\_child} + AT_{nc\_adult}} * \frac{1}{RfD}$$

where:
HI_c = Hazard Index Child only (unitless)
$HI_{a\&c}$ = Hazard Index Combined Child and Adult (unitless)
C_f = Chemical concentration in fish tissue (mg/kg) (calculated in PRAM)
IR_c = Fish ingestion rate in children (kg/day) (site-specific, daily average value)
IR_a = Fish ingestion rate in adults (kg/day) (site-specific, daily average value)
FI = Fraction of Fish Ingested (unitless) (site-specific value)
EF = Exposure frequency (days/year) (default value of 365 days/year; RME and CTE)
ED_c = Exposure duration for children (years) (default value of 6 years; RME and CTE)
ED_a = Exposure duration for adults (years) (default value of 3 years CTE; 24 years RME)
BW_c = Body weight of a child (kg) (default value of 15 kg; RME and CTE)
BW_a = Body weight of an adult (kg) (default value of 70 kg; RME and CTE)
AT_{nc_child} = Averaging time for non-carcinogens, child (days/year) (default value of 365 days/year * ED_c; RME and CTE)
AT_{nc_adult} = Averaging time for non-carcinogens, adult (days/year) (default value of 365 days/year * ED_a; RME and CTE)
RfD = Oral Reference dose (2E-5 mg/kg-day, RME; 4.5E-5 mg/kg-day, CTE)

Cancer risk, based on child exposure is presented in equation 133, and combined child and adult exposure, is presented in equation 134.

$$(133) \quad CR = \frac{C_f * IR_c * FI * EF * ED_c}{BW_c * AT_c} * SF$$

$$(134) \quad CR = \frac{C_f * EF * FI * (\frac{IR_c * ED_c}{BW_c} + \frac{IR_a * ED_a}{BW_a})}{AT_c} * SF$$

where:
CR = Cancer risk (unitless)
AT_c = Averaging time for carcinogens (days) (default value of 25,550 days)
SF = Cancer slope factor (2.0 $[\text{mg/kg-day}]^{-1}$ RME; 1.0 $[\text{mg/kg-day}]^{-1}$ CTE)

Exposure parameters used in the ex-ORISKANY risk calculations are provided below:

Risk Inputs	Adult		Child	
	RME	CTE	RME	CTE

Ingestion Rate (kg/day)	0.0261	0.0072	0.0093	0.0026
Fractional Intake (unitless)	0.17	0.25	0.17	0.25
Exposure Frequency (days/year)	365	365	365	365
Exposure Duration (years)	24	3	6	6
Body Weight (kg)	70	70	15	15
Averaging Time Non-Cancer (days)	8,760	1,095	2,190	2,190
Averaging Time Cancer (days)	25,550	25,550	25,550	25,550
Reference Dose (mg/kg-day)	2.0E-5	4.5E-5	2.0E-5	4.5E-5
Slope Factor $(mg/kg\text{-}day)^{-1}$	2.0	1.0	2.0	1.0

The PRAM risk characterization module generates cancer risks and non-cancer hazards from ingestion of representative fish species, based on the above risk modeling algorithms. Example site-specific output reports applicable to the ex-ORISKANY artificial reef site are presented in Appendix H.

4.5 UNCERTAINTY

Section 2 presents a comprehensive discussion of uncertainties associated with PRAM, including a discussion of sensitivity analysis for parameters in the abiotic and biotic-food web modules. This section focuses on uncertainties in the risk characterization module in PRAM. In-depth discussion of data uncertainty is presented in Sections 2 and 3.

4.5.1 Scenario Uncertainty

The PRAM risk characterization module assumes long-term fish ingestion by anglers (30 years based on combined child and adult exposure) and child exposure only (6 years). PRAM does not consider other exposure scenarios, such as dermal exposure and incidental ingestion of environmental media (water, suspended solids, and sediments), which are insignificant or improbable. These exposure scenarios are likely to be applicable to recreational divers and not anglers. Detailed discussion of why these scenarios do not pose a health concern is presented in the TDM Documentation (NEHC/SSC-SD, 2005).

The fish ingestion scenario is judged to be reasonable, yet conservative, because of the following:

- Anglers generally move around and about an artificial reef, catching fishes of various age and sizes, and keeping them if they are above the legal limit.

Fishing pressure is likely to reduce the number of older fish associated with the sunken reef that would be expected to bioconcentrate and bioaccumulate the largest amount of PCBs.

- PRAM calculates risks from ingestion of representative pelagic, benthic, and reef species. Each risk estimate assumes long-term ingestion of a single species, and those individual risk estimates are presented as the risk outputs. The highest estimated risks would be based on the species with the greatest concentration of PCBs. In reality, individuals are likely to consume various species, based on what they catch. Thus any high-end estimate based on ingestion of the single species with greatest PCB concentrations should be considered highly conservative.

- The FI term was based on a survey conducted by ECMRD on anglers, which posed hypothetical questions of how likely they would be to fish at the ex-ORISKANY and the amount of fish they might ingest from catches there. As with any survey of this kind, it was selective, rather than random, and was targeted to the group that would most likely be exposed. Use of this FI term is likely to overestimate risks for most anglers who won’t fish the reef on a regular basis.

- Many species of fish migrate from reef to reef, or are displaced from a reef during disturbances such as storm events/hurricanes. Therefore, the fish caught at an artificial reef may or may not spend a significant portion of their lives at that reef. The data (biota concentration) predicted by PRAM assumes the fish reside their entire lives at a reef. Thus the exposure point concentrations used in the risk characterization module may be biased high.

- PRAM does not consider background risks, i.e., the PCB concentrations; therefore, the risks predicted by the model are solely from the sunken vessel. If fishes migrating to a reef have already had PCB exposure, the actual fish PCB concentrations and associated risks may be higher than the predicted values. However, unless this other source of exposure is relatively close to the reef, it is unlikely to be a major contributor to the overall PCB concentrations of the reef community (i.e., the greater the distance of a secondary source of PCBs, the fewer reef fish that are likely to have originated from that alternative source area).

- The risk characterization module of PRAM calculates risks based on the whole body total PCB concentrations predicted by the biotic-food web module. It is most likely that anglers fillet and grill or pan-fry the fish. This preparation and cooking process may result in lower PCB concentrations in the fish ingested (and therefore lower risks) than those predicted by PRAM. Also, it is assumed that PCBs ingested are 100% available.

4.5.2 Parameter Uncertainty

The parameter uncertainty is associated with the input value and assumptions that are used behind the parameter. These parameters include biota concentrations (predicted by the biotic-food web module), exposure parameters such as exposure duration, frequency, body weight, and averaging time, and the toxicity value. With respect to biota concentration, the abiotic module is assumed to receive PCB releases indefinitely, i.e., without depletion (release rate was selected as a conservative constant release rate for modeling a steady-state condition). This conservativeness is likely to bias in biota concentration high, and thus the risks high. Although reasonable maximum exposure and central tendency exposure values are used in PRAM, input to each parameter may actually be a range of values. To fully characterize parametric uncertainty, a stochastic method such as Monte Carlo Simulations should be employed. The PRAM risk characterization module currently does not have that capability and therefore cannot present a spectrum of risks and hazards that reflects the variability of the underlying parameters. Therefore, we recommend that users and decision makers using PRAM compare the RME and CTE risks, as a means to judge the impact of variability or distribution of risks and hazards. As an example, the toxicity values were based on certain commercial PCB mixtures of aroclors, which may differ from those actually present. Hence the toxicity value provided by IRIS contains uncertainty that could not be easily ascertained.

4.5.3 Modeling Uncertainty

PRAM is a modeling tool, and as such, it employs known and documented algorithms and concepts that are based on good science and logic. Although developed as a predictive tool, it has not undergone extensive testing and validation. This does not mean it is not useful as a risk management tool. USEPA typically uses environmental fate and transport models and risk assessment models in their risk management process, yet, few have been field validated or tested. Overall, the modeling assumptions are generally conservative in nature. The use of multiple conservative or reasonably conservative assumptions in PRAM may result in the risks predicted to be in the realm of "theoretical upperbound" (i.e., overestimated) rather than reflecting actual risks (which could only be estimated by long-term environmental monitoring).

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TABLES

Table 1

Summary of Analysis of PCB Release Rate (Leachate) Data for Materials Found Onboard Ex-US Navy Vessels (Adapted from R. George, SSC-SD, 2004)

Rates are presented as ng PCB/g PCB/g Material/day	Mono-chlorobiphenyls	Di-chlorobiphenyls	Tri-chlorobiphenyls	Tetra-chlorobiphenyls	Penta-chlorobiphenyls	Hexa-chlorobiphenyls	Hepta-chlorobiphenyls	Octa-chlorobiphenyls	Nona-chlorobiphenyls	Deca-chlorobiphenyls
Aluminized Paint										
PCB = 0.04%										
Maximum Rate	0	0	261	1165	2240	1333	7191	0	0	0
Median Rate	0	0	0	283	1150	0	0	0	0	0
Maximum Occurs -	---	---	21 days	7-days	21-days	71-days	1-day	---	---	---
No. Detections	0	0	1	13	10	5	3	0	0	0
No. Non-detections	15	15	14	2	5	10	12	15	15	15
Regression Analysis										
ln(Intercept)	---	---	---	8.09E+00	9.74E+00	8.69E+00	8.85E+00	---	---	---
Slope	---	---	---	-4.96E-01	-5.70E-01	-3.69E-01	-7.19E-01	---	---	---
alpha	---	---	---	1.92E-03	1.67E-01	3.88E-01	1.37E-01	---	---	---
r2	---	---	---	0.5985	0.2538	0.2472	0.9546	---	---	---
rate at 2-years	---	---	SD	123	NS	NS	NS	---	---	---
Rate used for the PRAM	0	0	261	123	2240	1333	7191	0	0	0
Electrical Cable										
PCB = 0.12%										
Maximum Rate	0	203	1.14	38.8	73	24.1	14.7	0	1.51	0.84
Median Rate	0	0	0	23	42	0	0	0	0	0
Maximum Occurs -	---	6-days	125-days	40-days	40-days	125-days	6-days	---	125-days	125-days
No. Detections	0	0	1	13	10	5	3	0	0	0
No. Non-detections	15	15	14	2	5	10	12	15	15	15
Regression Analysis										
ln(Intercept)	---	7.11E+00	---	5.60E-01	5.93E+00	7.61E+00	4.00E+00	---	---	---
Slope	---	-1.16E+00	---	-2.62E-01	-4.62E-01	-9.45E-01	-6.10E-01	---	---	---
alpha	---	3.22E-01	---	3.30E-02	3.05E-02	1.20E-01	2.52E-01	---	---	---
r2	---	0.7655	---	0.3794	0.3880	0.7741	0.8515	---	---	---
rate at 2-years	---	NS	---	15.7	18.0	NS	NS	---	---	---
Rate used for the PRAM	0	203	1.14	15.7	18.0	24.1	14.7	0	1.51	0.84

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Rates are presented as ng PCB/g PCB/g Material/day	Mono-chlorobiphenyls	Di-chlorobiphenyls	Tri-chlorobiphenyls	Tetra-chlorobiphenyls	Penta-chlorobiphenyls	Hexa-chlorobiphenyls	Hepta-chlorobiphenyls	Octa-chlorobiphenyls	Nona-chlorobiphenyls	Deca-chlorobiphenyls
Bulkhead Insulation										
PCB = 0.044%										
Maximum Rate	0	8209	8259	158137	286990	53159	34568	0	0	0
Median Rate	0	0.0	2091	53427	95598	17305	0	0	0	0
Maximum Occurs -	---	14-days	7-days	21-days	21-days	69-days	1-day	---	---	---
No. Detections	0	8	16	16	16	15	6	0	0	0
No. Non-detections	17	9	1	1	1	2	11	17	17	17
Regression Analysis										
ln(Intercept)	---	1.16E+01	1.00E+01	1.38E+01	1.46E+01	1.45E+01	9.97E+00	---	---	---
Slope	---	-1.51E+00	-4.85E-01	-5.89E-01	-6.21E-01	-8.69E-01	-4.24E-01	---	---	---
alpha	---	8.18E-04	4.14E-07	2.63E-05	6.54E-04	1.37E-03	2.43E-02	---	---	---
r2	---	0.8646	0.8593	0.8117	0.6672	0.6976	0.7568	---	---	---
rate at 2-years	---	5.36	944	20704	37917	6762	1303	---	---	---
Rate used for the PRAM	0	5.36	944	20704	37917	6762	1303	0	0	0
Rubber Material (also used for ventilation gaskets)										
PCB = 0.16%										
Maximum Rate	184	1267	239	922	638	0	167503	0	0	0
Median Rate	57.1	43.5	82.9	284	248	0	0	0	0	0
Maximum Occurs -	7-days	14-days	14-days	14-days	69-days	---	<1 day	---	---	---
No. Detections	12	14	14	14	14	0	4	0	0	0
No. Non-detections	4	2	2	2	2	16	12	16	16	16
Regression Analysis										
ln(Intercept)	5.81E+00	7.09E+00	5.99E+00	8.50E+00	1.07E+01	---	7.40E+00	---	---	---
Slope	-3.17E-01	-6.55E-01	-2.97E-01	-5.36E-01	-9.95E-01	---	-8.78E-01	---	---	---
alpha	2.88E-08	7.83E-02	4.98E-02	2.22E-05	4.47E-03	---	7.51E-03	---	---	---
r2	0.9591	0.2552	0.3063	0.8007	0.6567	---	0.9850	---	---	---
rate at 2-years	41.4	NS	56.6	144	63.1	---	5.04	---	---	---
Rate used for the PRAM	41.4	1267	56.6	144	63.1	0	5.04	0	0	0

Table 1

Summary of Analysis of PCB Release Rate (Leachate) Data for Materials Found Onboard Ex-US Navy Vessels (Adapted from R. George, SSC-SD, 2004)

Rates are presented as ng PCB/g PCB/g Material/day	Mono-chlorobiphenyls	Di-chlorobiphenyls	Tri-chlorobiphenyls	Tetra-chlorobiphenyls	Penta-chlorobiphenyls	Hexa-chlorobiphenyls	Hepta-chlorobiphenyls	Octa-chlorobiphenyls	Nona-chlorobiphenyls	Deca-chlorobiphenyls
Aroclor 1254 (used for lubricants)										
PCB = 10%										
Maximum Rate	554	1576	1103	22679	26356	2636	71.7	0	0	0
Median Rate	83.2	340.3	344.2	5373	2778	347	0	0	0	0
Maximum Occurs -	1-day	1-day	69-days	69-days	69-days	69-days	230-days	---	---	---
No. Detections	14	14	14	14	13	12	1	0	0	0
No. Non-detections	1	1	1	1	2	3	14	15	15	15
Regression Analysis										
ln(Intercept)	6.96E+00	7.80E+00	1.05E+01	1.44E+01	1.57E+01	1.31E+01	---	---	---	---
Slope	-5.17E-01	-4.02E-01	-9.18E-01	-1.12E+00	-1.40E+00	-1.30E+00	---	---	---	---
alpha	1.97E-06	1.70E-06	5.02E-04	7.49E-04	1.57E-03	4.18E-03	---	---	---	---
r2	0.8581	0.8614	0.8407	0.8218	0.7811	0.7131	---	---	---	---
rate at 2-years	34.7	172	89.7	1082	660	94	---	---	---	---
Rate used for the PRAM	34.7	172	89.7	1082	660	94	71.7	0	0	0

where:

SD = A significant number of detections were not observed to perform statistical analyses. Maximum measured rate is used.

NS = Statistical regression not significant. Maximum measured rate is used.

Table 2

Physical-Chemical Parameters for PCB Homologs Used in the Prospective Risk Assessment Model (PRAM)

Chemical Parameter	Source	Mono-CB	Di-CB	Tri-CB	Tetra-CB	Penta-CB	Hexa-CB	Hepta-CB	Octa-CB	Nona-CB	Deca-CB
log10Kow =	1	4.474	5.236	5.521	5.922	6.4951	6.9761	7.19	7.696	8.351	9.603
log10Koc =	2	3.66	4.06	4.63	4.65	4.94	6.08	6.34	6.45	6.97	7.94
log10Kdoc =	3	3.34	4.11	4.39	4.79	5.36	5.85	6.06	6.57	7.22	8.47
Molecular Weight (g/mol)	4	188.65	223.1	257.54	291.99	326.43	360.88	395.32	429.77	464.21	498.66
Solubility (mg/L)	5	2.91E+00	6.78E-01	8.14E-02	6.67E-02	2.61E-02	9.50E-04	2.30E-04	2.11E-08	4.02E-09	1.69E-10
Solubility (mol/m^3)		1.54E-02	3.04E-03	3.16E-04	2.28E-04	8.00E-05	2.63E-06	5.82E-07	4.91E-11	8.65E-12	3.38E-13
Vapor Pressure (Pa)	6	6.32E-01	1.41E-01	2.44E-02	2.08E-02	2.96E-03	3.43E-03	2.56E-04	8.65E-05	2.77E-05	1.41E-05
Henry's ($Pa\text{-}m^3/mol$) VP/Sol	7	4.10E+01	4.65E+01	7.70E+01	9.10E+01	3.70E+01	1.30E+03	4.40E+02	1.76E+06	3.20E+06	4.18E+07

1 Based on statistical analysis of data reported by Eisler and Belisle (1996)

2 Geomeans from Chou and Griffin (1986)
hepta, octa, nona, and deca-CB are based on regression presented by Lyman (1995; equation #10)

3 Per USEPA (2002) Kow Kdoc ratio (0.074)

4 Sawhney (1986) in PCBs and the Environment

5 Geomeans from Chou and Griffin (1986) in PCBs and the Environment
hepta, octa, nona, and deca-CB were estimated using Equation #1 in Lyman (1995)

6 Based on statistical analysis of data reported by Fiedler (2001),
mono, hepta, octa, nona, and deca-CB based on the geomean of data reported by Oberg (2001)

7 Calculated (VP/sol) per Lyman (1995, equation #21)

Table 3

Example PCB Degradation Rates in Surface Water

	Biodegradation Rate	Units	Water type	Reference	Half life	Units	Water type	Reference
Homolog								
Monochlorobiphenyl	2 - 5	days for 50% biodegradation	Fresh	Bailey et al. 1983	1.4 - 4.9	days	Fresh (Lake Michigan)	Neely 1983
	7.0E-08	nmol/cell/hour	Bacterial culture with Acinetobacter	Furukawa et al. 1978	2 - 3	days	Fresh	Bailey et al. 1983
Dichlorobiphenyl	2 - 3	days	Fresh	Bailey et al. 1983	2 - 3	days	Fresh	Bailey et al. 1983
	6.0E-08	nmol/cell/hour	Bacterial culture with Acinetobacter	Furukawa et al. 1978				
Trichlorobiphenyl	5.0E-08	nmol/cell/hour	Bacterial culture with Acinetobacter	Furukawa et al. 1978				
Tetrachlorobiphenyl	2.5E-08	nmol/cell/hour	Bacterial culture with Acinetobacter	Furukawa et al. 1978				
	0	98 day river dieaway test	Fresh	Bailey et al. 1983				
Pentachlorobiphenyl								
Hexachlorobiphenyl	1.5E-05	$hour^{-1}$	Not given	Mackay and Patterson 1991				

Table 3

Example PCB Degradation Rates in Surface Water

	Biodegradation Rate	Units	Water type	Reference	Half life	Units	Water type	Reference
Commercial Aroclor Mixtures								
Aroclor 1221	3E-09 to 3E-12	ml/cell/hour	transformation rate by bacteria in water	Mabey et al. 1982				
Aroclor 1232	3E-09 to 3E-12	ml/cell/hour	transformation rate by bacteria in water	Mabey et al. 1982				
Aroclor 1016	3E-09 to 3E-12	ml/cell/hour	transformation rate by bacteria in water	Mabey et al. 1982	9.9	hours	At 1m depth in 1m^3 water	Paris et al. 1978
Aroclor 1242	3E-09 to 3E-12	ml/cell/hour	transformation rate by bacteria in water	Mabey et al. 1982	12	hours	Not given	Paris et al. 1978
					12	hours	Volatilization half life at 1m depth in 1m^3 water	Mackay and Leinonen 1975
Aroclor 1248	3E-09 to 3E-12	ml/cell/hour	transformation rate by bacteria in water	Mabey et al. 1982	10	hours	Volatilization half life at 1m depth in 1m^3 water	Mackay and Leinonen 1975
Aroclor 1254	3E-09 to 3E-12	ml/cell/hour	transformation rate by bacteria in water	Mabey et al. 1982	10	hours	Volatilization half life at 1m depth in 1m^3 water	Mackay and Leinonen 1975
Aroclor 1260	0	12 weeks	Biodegradation rate, water type not given	Oloffs et al. 1972	7.53	hours	Evaporation half life in 1m water	Mackay and Leinonen 1975
	3E-09 to 3E-12	ml/cell/hour	transformation rate by bacteria in water	Mabey et al. 1982	10	hours	Volatilization half life at 1m depth in 1m^3 water	Mackay and Leinonen 1975
					52	days	Volatilization half life in river water	Oloffs et al. 1972

Table 3

Example PCB Degradation Rates in Surface Water

	Biodegradation Rate	Units	Water type	Reference	Half life	Units	Water type	Reference
Individual Congeners								
Biphenyl	9.3 - 9.8	nmol/L-day	Marine with initial water conc. of 4.4-4.7μmol/L	Reichardt et al. 1981	1.5	days	Fresh	Bailey et al. 1983
	3.2	nmol/L-day	Marine with initial water conc. of 2.9 μmol/L	Reichardt et al. 1981				
2-chlorobiphenyl	1.1 - 3.7E-04	day^{-1}	Sunlight photolysis rate in unspecified surface water	Dulin et al. 1986	1.4	days	Fresh	Neely 1983
	63	$year^{-1}$	Microbial degradation rate in unspecified surface water	Wong and Kaiser 1975	2 - 3.5	days	50% degradation of 1-100 μg/L in river dieaway test	Bailey et al. 1983
	4.1	nmol/L-day	Marine with initial water conc. of 1.5 μmol/L	Reichardt et al. 1981	18	years	Photolysis half life in unspecified surface water	Dulin et al. 1986
	1.2	nmol/L-day	Marine with initial water conc. of 4.5 μmol/L	Reichardt et al. 1981				
	1.1	μg/ml/day	Degradation rate in fresh water with 30 μg/ml initial conc.	Kong and Sayler 1983				
3-chlorobiphenyl	2.6	nmol/L-day	Marine with initial water conc. of 3.6 μmol/L	Reichardt et al. 1981	3 - 4	days	50% degradation of 1-100 μg/L in river dieaway test	Bailey et al. 1983
	1.1	μg/ml/day	Degradation rate in fresh water with 30 μg/ml initial conc.	Kong and Sayler 1983				
4-chlorobiphenyl	0.115 - 2.3E-04	day^{-1}	Sunlight photolysis rate in unspecified surface water	Dulin et al. 1986	4.9	days	Fresh	Neely 1983
	38	$year^{-1}$	Microbial degradation rate in unspecified surface water	Wong and Kaiser 1975	8.2	years	Photolysis half life in unspecified surface water	Dulin et al. 1986
	3.1	nmol/L-day	Marine with initial water conc. of 2.9 μmol/L	Reichardt et al. 1981	2 - 5	days	50% degradation of 1-100 μg/L in river dieaway test	Bailey et al. 1983
	2.0	μg/ml/day	Degradation rate in fresh water with 30 μg/ml initial conc.	Kong and Sayler 1983				

Table 3

Example PCB Degradation Rates in Surface Water

	Biodegradation Rate	Units	Water type	Reference	Half life	Units	Water type	Reference
Individual Congeners (continued)								
2,2'-dichlorobiphenyl	0.65	$year^{-1}$	Not given, microbial degradation 1st order rate constant	Furukawa et al. 1978	34.5	days	Fresh	Neely 1983
2,4-dichlorobiphenyl	<2.0E-08	sec^{-1}	Sunlight photolysis rate constant in unspecified surface water	Dulin et al. 1986	>400	days	Photolysis half life in unspecified surface water	Dulin et al. 1986
4,4'-dichlorobiphenyl					57.5	days	Fresh	Neely 1983
2,2',5-trichlorobiphenyl					43.1	days	Fresh	Neely 1983
2,4,4'-trichlorobiphenyl	2.2E-08	sec^{-1}	Sunlight photolysis rate constant in unspecified surface water	Dulin et al. 1986	133	days	Photolysis half life in unspecified surface water	Dulin et al. 1986
2,2',4,4'-tetrachlorobiphenyl	0	98 days	Fresh, river dieaway test	Bailey et al. 1983	49.2	days	Fresh	Neely 1983
	0.055 - 0.553	day^{-1}	Summer sunlight photolysis rate constant in unspecified surface water	Dulin et al. 1986	13	days	Summertime photolysis half life in unspecified surface water	Dulin et al. 1986
	5E-08	day^{-1}	Winter sunlight photolysis rate constant in unspecified surface water	Dulin et al. 1986	170	days	Wintertime photolysis half life in unspecified surface water	Dulin et al. 1986
2,2',5,5'-tetrachlorobiphenyl	0.1	$year^{-1}$	Pseudo first order rate constant in unspecified surface water	Furukawa et al. 1978	19.7	days	Fresh	Neely 1983
3,3',4'4'-tetrachlorobiphenyl					805	days	Fresh	Neely 1983
2,2',3,4,5-pentachlorobiphenyl	0.005	$year^{-1}$	Pseudo first order rate constant in unspecified surface water	Furukawa et al. 1978	108	days	Fresh	Neely 1983
2,2',4,5,5'-pentachlorobiphenyl	1.5E-08	nmol/cell/hour	Bacterial culture with Acinetobacter	Furukawa et al. 1978				
2,2',4,4',5,5'-hexachlorobiphenyl					25 - 53	minutes	Aqueous solution purged at flow rate of 1 L/min	Coates 1984

Table 3

Example PCB Degradation Rates in Surface Water

Literature cited for PCB degradation rates in surface water

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Secondary sources for literature cited above

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Environmental Fate Data Base. Managed by Syracuse Research Corporation with suppport from the U.S. Environmental Protection Agency, DuPont and Procter & Gamble. Internet address: http://esc.syrres.com/efdb.htm

Table 4
Fugacity-Based PCB Transport Coefficients Used in the PRAM

Compartment	Process	Notation	Solution
1 Air	diffusion from air to upper water column	D_V	$D_V = 1/\{[1/(A_{12}*U_{12}*Z_A)]+[1/(A_{12}*U_{21}*Z_W)]\}$
	rain deposition	D_{QW}	$D_{QW} = A_{12}*U_Q*Z_W$
	wet particle deposition into upper water column	D_{DW}	$D_{DW} = A_{12}*\phi_{1AE}*U_Q*Z_{1AE}$
	dry particle deposition into upper water column	D_{PW}	$D_{PW} = A_{12}*\phi_{1AE}*U_P*Z_{1AE}$
	advection of bulk air out of system	D_{A1}	$D_{A1} = G_A*Z_1$
2 Upper Water Column	diffusion from water to air	D_V	$D_V = 1/\{[1/(A_{12}*U_{12}*Z_A)+[(1/(A_{12}*U_{21}*Z_W)]\}$
	diffusion from upper water column to lower water column	D_W	$D_W = 1/\{[1/(A_{23}*1.728*Z_W)]+[1/(A_{23}*1.728*Z_W)]\}$
	advection of bulk water out of the system	D_{A2}	$D_{A2} = G_{W2}*Z_2$
	degradation in bulk water	D_{R2}	$D_{R2} = K_w*V_{2W}*\phi_{2W}*Z_W$
3 Lower Water Column	diffusion from lower water column to upper water column	D_W	$D_W = 1/\{[1/(A_{23}*1.728*Z_W)]+[1/(A_{23}*1.728*Z_W)]\}$
	diffusion from lower water column to sediment bed	D_Y	$D_Y = 1/\{[(1/A_{43}*U_{34}*Z_W)+[(1/(A_{34}*U_{43}*Z_W)]\}$
	deposition of suspended solids onto sediment bed	D_{DX}	$D_{DX} = A_{34}*U_{DX}*\phi_{3SS}*Z_{SS}$
	advection of bulk water out of the system	D_{A3}	$D_{A3} = G_{W3}*Z_3$
	degradation in bulk water	D_{R3}	$D_{R3} = K_w*V_{3W}*\phi_{3W}*Z_W$
4 Sediment Bed	diffusion from sediment bed into lower water column	D_Y	$D_Y = 1/\{[(1/A_{43}*U_{34}*Z_W)+[(1/(A_{34}*U_{43}*Z_W)]\}$
	re-suspension of sediment into lower water column	D_{RX}	$D_{RX} = A_{34}*U_{RX}*\phi_{3SD}*Z_{SD}$
	degradation in bulk sediment	D_{R4}	$D_{R4} = K_w*V_{4W}*\phi_{4W}*Z_W$
	sediment burial (advection) out of system	D_B	$D_B = A_4*U_B*\phi_{3SD}*Z_{SD}$
5 Vessel Interior	advection of bulk water into lower water column	D_{A5}	$D_{A5} = G_{W5}*Z_5$
Inter-compartment Transport Coefficients	Air to water	$D_{12} = D_V + D_{QW} + D_{DW} + D_{PW}$	
	Upper water column to air	$D_{21} = D_V$	
	Upper water column to lower water column	$D_{23} = D_W$	
	Lower water column to upper water column	$D_{32} = D_W$	
	Lower water column to sediment bed including suspended solids	$D_{34} = D_Y + D_{DX}$	
	Sediment bed to lower water column including resuspension of sediment	$D_{43} = D_Y + D_{RX}$	
	Sunken vessel to lower water column	$D_{53} = D_{A5}$	

ΣD-air =	$D_{12} + D_{A1} = DT_1$
ΣD-upper water column =	$D_{21} + D_{23} + D_{A2} + D_{R2} = DT_2$
ΣD-lower water column =	$D_{32} + D_{34} + D_{A3} + D_{R3} = DT_3$
ΣD-sediment bed =	$D_{43} + D_{R4} + D_B = DT_4$

Note: See Figures 4 and 6 for additional information on process/compartment interaction.

Table 5

Food Web Diet Compositions Assumed for the PRAM and the ex-ORISKANY Memorial Reef

	Suspended Solids (Epilimnion)	Suspended Solids (Hypolimnion)	Sediment[7]	Phytoplankton	Zooplankton	Pelagic Planktivore	Attached Algae	Reef Sessile Filter Feeder	Invertebrate Omnivore[3]	Reef Invertebrate Forager	Reef Vertebrate Forager	Infaunal Benthos	Epifaunal Benthos	Benthic Forager	Total
Pelagic (open water associated organisms)															0%
Zooplankton (TL-II)	15%[1]	15%[1]		70%											100%
Planktivore (TL-III)	0%	0%		0%	100%			0%					0%		100%
Piscivore (TL-IV)				0%	10%	90%		0%	0%	0%	0%		0%	0%	100%
Benthic (sediment associated organisms)															
Infaunal Macroinvertebrate (TL-II)			50%[2]	30%[2]	20%[2]		0%								0%
Epifaunal Invertebrate (TL-II)		0%	25%[2]	30%[2]	20%[2]		0%					25%[2]			100%
Benthic Forager (TL-III)		0%	5%	0%	0%	0%	0%					50%	45%		100%
Benthic Predator (TL-IV)		0%	2%	0%	0%	0%						20%	20%	58%	100%
Reef (reef associated organisms)															
Sessile filter feeder (TL-II)	0%	10%		80%	10%		0%								100%
Invertebrate Omnivore (TL-II)[3]	0%	0%		0%	0%		80%	20%					0%		100%
Invertebrate Forager (TL-III)		5%		0%	5%	5%	0%[4]	35%[4]	50%[4]			0%	0%		100%
Vertebrate Forager (TL-III)		0%		0%	0%[5]	19%[6]	0%[5]	19%[6]	15%[6]	22%[6]		12.5%[6]	12.5%[6]	0%	100%
Reef Predator (TL-IV)		0%		0%	0%	0%	0%	0%	0%	15%[6]	60%[6]	8%[6]	8%[6]	8%[6]	99%

Notes:

[1] In recognition of the splitting time spent below the pycnocline, the dietary fractions have been adjusted to account for feeding below the pycnocline.

[2] In recognition of comments made and in consideration that a higher sediment ingestion rate would result in a more conservative exposure level, the compromised dietary fractions are presented.

[3] Based on a deductive evaluation of the potential PCB transfer pathways within the reef community, an invertebrate omnivore (e.g., echinoderm), was considered more significant than mobile reef planktivores.

[4] Based on comments made by J. Dodrill.

[5] Based on addition of invertebrate omnivore (TL-II) to the reef food web.

[6] Based on comments made by Robert Turpin indicating that vertebrate reef foragers and predators obtain a significant portion of their energy budget from the benthos.

[7] The term "sediment" refers to any material within the sediment bed that supplies the biological energy input, including detritus/Particulate Organic Matter.

Table 6

Food Web Water Exposure Values Assumed for the PRAM and the ex-ORISKANY Memorial Reef (Modified with Comments from Biology Technical Working Group; Revised, 12/31/04)

	Upper Water Column	Lower Water Column	Vessel Interior	Sediment Pore Water	Total
Pelagic Community					
Phytoplankton (TL-I)	100%				100%
Zooplankton (TL-II)	50%	50%[3]			100%
Planktivore (TL-III)	80%	20%			100%
Piscivore (TL-IV)	80%	20%			100%
Reef / Vessel Community					
Attached algae (TL-I)		100%			100%
Sessile filter feeder (TL-II)	0%	100%	0%[1]		100%
Invertebrate Omnivore (TL-II)[2]	0%	80%	20%		100%
Invertebrate forager (TL-III)	0%	70%	30%		100%
Vertebrate forager (TL-III)	0%	70%	30%		100%
Predator (TL-IV)	0%	80%	20%		100%
Benthic Community					
Infaunal macro-invertebrate (TL-II)	0%	20%		80%	100%
Epifaunal invertebrate (TL-II)	0%	50%		50%	100%
Forager (TL-III)	0%	75%		25%	100%
Predator (TL-IV)	0%	90%		10%	100%

Notes:

TL stands for Trophic Level

[1] This value is set to zero, per response to comments, which reflects our position that a vessel interior community is unlikely, and if existent, would represent a negligible portion of the overall reef community biomass.

[2] Based on a deductive evaluation of the potential PCB transfer pathways within the reef community, an invertebrate omnivore (e.g., echinoderm), was considered more significant than mobile reef planktivores.

[3] In recognition of the splitting time spent below the pycnocline, the dietary fractions have been adjusted to account for feeding below the pycnocline.

Table 7

Biological Parameters for Food Web Components Within the PRAM

	Representative Species	Body Weight (kg)[a]	Lipid (%-dw)	Moisture (%)[b]	Caloric Density (kcal/g-dw)[b]	Fraction Metabolizable Energy from Gross[b]	Production[e] (% of total)	Respiration[e] (% of total)	Excretion[e] (% of total)
Pelagic Community									
Phytoplankton (TL-I)	algae	---	10.3%[c]	84%	2.36	0.60	---	---	---
Zooplankton (TL-II)	copepods	0.000005	22.0%[c]	76%	3.6	0.65	18%[c]	24%	58%
Planktivore (TL-III)	herring	0.05	28.1%[d1]	75%	4.9	0.70	20%	60%	20%
Piscivore (TL-IV)	jack	0.5	28.1%[d1]	75%	4.9	0.70	20%	60%	20%
Reef / Vessel Community									
Attached algae (TL-I)	algae	---	10.3%[c]	84%	2.36	0.60	---	---	---
Sessile filter feeder (TL-II)	bivalves (w/o shell)	0.05	4.96%[d2]	82%	4.6	0.65	28%	31%	41%
Grazing / foraging omnivore (TL-II)	urchin	0.05	29.0%[d6]	82%[f]	4.6[f]	0.65	7%[g]	25%[g]	68%[g]
Invertebrate forager (TL-III)	crab	1	9.18%[d3]	74%	2.7	0.65	28%	59%	13%
Vertebrate forager (TL-III)	triggerfish	1	28.1%[d1]	75%	4.9	0.70	20%	60%	20%
Predator (TL-IV)	grouper	1.5	28.1%[d1]	75%	4.9	0.70	20%	60%	20%
Benthic Community									
Infaunal invertebrate (TL-II)	polychaete	0.01	5.98%[d4]	84%	4.6	0.65	71%[g]	26%[g]	3%[g]
Epifaunal invertebrate (TL-II)	nematode	0.01	5.98%[d4]	84%	4.6	0.65	31%	19%	50%
Forager (TL-III)	lobster	2	9.18%[d3]	74%	2.7	0.65	28%	59%	13%
Predator (TL-IV)	flounder	3	22.0%[d5]	75%	4.9	0.70	20%	60%	20%

Notes:

a = based on professional judgment for typical member of trophic level

b = values obtained from USEPA 1993

c = obtained from Parsons et al. 1979 (average of algae values in Table 6; zooplankton from Table 14 in Parsons et al. 1979)

d = obtained from USACE 2004 (http://ered1.wes.army.mil/cgi-bin/LipidOrgMean.exe)

1 = midwater fish wet weight converted using % moisture presented here

2 = marine / estuarine mollusks

3 = marine crustecea

4 = marine / estuarine worms

5 = bottom fish

6 = echinoderms

e = derived from energy budgets reported by Welch (1968), Table reflects combined energy loss due to fecal (F) and urinary (U) excretion as total excretion (EX)

f = assumed to equal that of bivalves without the shell

g = obtained from Parsons et al. 1979 Table 38

TL = trophic level

dw = dry weight

Table 8

Temperature and Body Weight Dependent Oxygen Consumption Regressions for the Biological Components Within the PRAM

	Biota Type	α	β_1	β_2	Reference
Pelagic Community					
Pelagic zooplankton	copepod	0.00638	0	0.0399	Derived from Altman and Dittmer (1971)
Pelagic planktivore	herring	0.00330	-0.227	0.0548	Hewett and Johnson (1992)
Pelagic Predator	jack	0.001118602	-0.55	0.12	Derived by Barber (2004)*
Reef / Vessel Community					
Reef/Vessel sessile filter feeder	clam	0.012	0	0.036	Connolly (1991)**
Reef/Vessel omnivorous invertebrate	urchin	0.00068	0	0.0792	Derived from Altman and Dittmer (1971)
Reef/Vessel invertebrate forager	crab	0.00116	0	0.0712	Derived from Altman and Dittmer (1971)
Reef/Vessel vertebrate forager	triggerfish	0.01518	-0.415	0.061	Derived by Barber (2004)*
Reef/Vessel predator	grouper	0.00279	-0.355	0.0811	Kline (2004)
Benthic Community					
Benthic infaunal invertebrate	polychaete	0.00168	0	0.0710	Derived from Altman and Dittmer (1971)
Benthic epifaunal invertebrate	nematode	0.00168	0	0.0710	Derived from Altman and Dittmer (1971)
Benthic forager	lobster	0.0035	-0.13	0.066	Connolly (1991)
Benthic predator	flounder	0.0046	-0.24	0.067	Connolly (1991)

Respiration rate from the following equation has units of day^{-1}.

$$r\left[\frac{1}{day}\right] = \alpha W\left[g\right]^{\beta_1} e^{\beta_2\left(T\left[{}^{o}C\right]\right)}$$

where:
r = the oxygen consumption rate
W = organism body wet weight in grams
T = temperature in degrees Celsius
α = allometric intercept
e = the natural logarithm base
β_1, β_2 = allometric slopes for body weight and temperature, respectively
* = values provided by Barber were derived for an equation with different units and dimensions than the equation for r, therefore the values shown in the table have been adjusted by the methodology in the following footnote.
** = mussel parameters were considered most representative of a reef sessile filter feeder and were therefore selected for use in PRAM

Table 8

Temperature and Body Weight Dependent Oxygen Consumption Regressions for the Biological Components Within the PRAM

Adjustment of allometric parameters provided by Barber

The oxygen consumption rates used in PRAM are calculated in units of day^{-1}. Barber's allometric parameters are derived for an equation which calculates rates as milligrams of O_2 per hour. Since these two rates are not equivalent in either dimensions or units, an adjustment of Barber's parameters must be made before utilizing them in PRAM. The adjustment has been made as follows:

Given: $r\left[\frac{1}{day}\right] = \left(\alpha_{1PRAM} W[g]^{\beta_{1PRAM}} e^{\beta_{2PRAM}(T[^{\circ}C])}\right)$ and $r\left[\frac{mgO_2}{h}\right] = \left(\alpha_{1Barber} W[g]^{\beta_{1Barber}} e^{\beta_{2Barber}(T[^{\circ}C])}\right)$

(1) $$r\left[\frac{1}{day}\right] \times \left(\frac{2.67 gO_2}{gC}\right) \times \left(\frac{0.45 gC}{g_{dw}}\right) \times \left((1-f)\frac{g_{dw}}{g_{ww}}\right) = r\left[\frac{mgO_2}{h}\right] \times \left(\frac{1}{g_{ww}}\right) \times \left(\frac{gO_2}{1000 mgO_2}\right) \times \left(\frac{24h}{day}\right)$$

Where f = fraction moisture value from Table 8

(2) $$r\left[\frac{1}{day}\right] = r\left[\frac{mgO_2}{h}\right] \times \left(\frac{1}{g_{ww}}\right) \times \left(\frac{24}{2.67 \times 0.45 \times (1-f) \times 1000}\right)$$

(3) $$\alpha_{PRAM} W[g]^{\beta_{1PRAM}} e^{\beta_{2PRAM}(T[^{\circ}C])} = \left(\alpha_{Barber} W[g]^{\beta_{1Barber}} e^{\beta_{2Barber}(T[^{\circ}C])}\right) \times \left(\frac{1}{g_{ww}}\right) \times \left(\frac{24}{2.67 \times 0.45 \times (1-f) \times 1000}\right)$$

(4) $$\alpha_{PRAM} W[g]^{\beta_{1PRAM}} e^{\beta_{2PRAM}(T[^{\circ}C])} = \left(\alpha_{Barber} W[g]^{\beta_{1Barber}-1} e^{\beta_{2Barber}(T[^{\circ}C])}\right) \times \left(\frac{24}{2.67 \times 0.45 \times (1-f) \times 1000}\right)$$

From equation 4, we can observe the following relationships between parameters

$$\alpha_{1PRAM} = \alpha_{1Barber}\left(\frac{24}{2.67 \times 0.45 \times (1-f) \times 1000}\right) \qquad \beta_{1PRAM} = \beta_{1Barber} - 1 \qquad \beta_{2PRAM} = \beta_{2Barber}$$

The parameters provided by Barber have been adjusted as follows:

		α_1	β_1	β_2
Snapper species (jack, f = 0.75)	Barber	0.014	0.45	0.12
	PRAM	0.0011186	-0.55	0.12
Interspecies (triggerfish, f = 0.75)	Barber	0.19	0.585	0.061
	PRAM	0.015181	-0.415	0.061

Table 9

Physical Boundaries and Conditions for the EX-ORISKANY Memorial Site

	Value	Units	Value	Units	Comments
Vessel					
Displacement [1]	27100	tons	27533600	kg	
Length [1]	888	ft	271	m	
Beam [1a]	120	ft	36.6	m	
Water depth [5]	212	ft	65	m	
Surface Water (all depths)					
Depth to the pycnocline [2]			15	m	Consensus of TWG
Suspended solids density [2]			1.5	g/cm^3	
Aerosol density [3]			1.19	g/cm^3	
Dissolved organic carbon density [2]			1	g/cm^3	
Suspended solids fraction organic carbon [4]			15%	percent	
Air					
Air temperature [5]			22.3	°C	
Active air space height above water column [3]			10	m	
Air current [6]	8.5	mph	13677	meters/hr	
Aerosol concentration [3]			2.38.E-14	g/cm^3	
Rainfall [7]			6.50E-04	m/day	Reference of 60 inches per year
Particle deposition rate [3]			10.8	m/hr	
Water above the pycnocline					
Temperature [5]			24.5	°C	
Dissolved oxygen [8]			6.12	mg/L	
Total suspended solids [3]			10	mg/L	
Dissolved organic carbon [4]			0.6	mg/L	
Water current [6]	0.5	knot	926	meters/hr	Consensus of TWG
Water below the pycnocline					
Temperature [4]			19.5	°C	
Dissolved oxygen [8]			6.12	mg/L	
Total suspended solids [2]			10	mg/L	
Dissolved organic carbon [4]			0.6	mg/L	
Water current [6]	0.5	knot	926	meters/hr	Consensus of TWG

Table 9

Physical Boundaries and Conditions for the EX-ORISKANY Memorial Site

	Value Units	Value Units	Comments
Water within the vessel interior			
Temperature [4]		19.5 °C	
Dissolved oxygen [9]		4.59 mg/L	
Total suspended solids [3]		10 mg/L	
Dissolved organic carbon [4]		0.6 mg/L	
Water current - inside the vessel to outside the vessel [10]		9.26 meters/hr	
Sediment bed			
Temperature [4]		19.5 °C	
Dissolved oxygen [9]		3.06 mg/L	
Dissolved organic carbon [11]		2 mg/L	
Sediment fraction organic carbon [4]		1% percent	
Sediment density [2]		1.5 g/cm3	
Sediment moisture [2]		10% percent	
Bio-active sediment depth [12]		0.1 m	
Sediment deposition rate [13]		0 m^3/m^2-day	
Sediment resuspension rate [13]		0 m^3/m^2-day	
Sediment burial rate [13]		0 m^3/m^2-day	

Notes:

1 = Based on Dictionary of American Naval Fighting Ships (online at http://www.hazegary.org/danfs/carriers/cv34.htm).

1a = Average between hull beam (93 ft) and flight deck beam (147.5 ft)

2 = Based on professional judgment

3 = Based on value used by Mackay and Paterson (1991)

4 = Typical or low-end value for oceans obtained from Parsons et al. 1979

5 = Yearly average at NOAA buoy # 42040 (online at http://www.ndbc.noaa.gov/station_history.phtml?station=42040).

6 = FFWCC 2004

7 = Based on a yearly average rainfall of 60 inches

8 = Based on Temperature (°C) and 90% saturation level (Spotte 1970)

9 = Assumes 75% of DO in water below pycnocline

10 = Assumed to be 1/10 of current of water within water column below pycnocline

11 = Upper limit for open ocean surface water obtained from Parsons et al. 1979

12 = Based on evidence obtained from Bosworth and Thibodeaux 1990

13 = Set at zero - assumes deposition and resuspension balance

Table 10

Summary of Statistical Analysis of PCB Concentrations in Materials Onboard the ex-ORISKANY

PCB-Containing Material (estimated and detected values are in mg/kg)	Statistical Method	Resultant Estimate	Statistical Method	Resultant Estimate	Number of Samples	Detection Frequency	Maximum Detection	Minimum Detection	Maximum Non-detection	Minimum Non-detection	Comment
Bulkhead Insulation	Jackknife Mean	2.15E+02	Jackknifed UCL	5.37E+02	32	56%	6100	5.5	5	5	There is a sufficient number of values for statistical analysis - the data were found to be non-normal, however, the bootstrap methods failed to normalize the dataset - use the Jackknife mean and UCL
Aluminized Paint	Jackknife Mean	1.26E+01	Jackknifed UCL	2.00E+01	7	57%	28	5.8	5	5	There is a sufficient number of values for statistical analysis - the data were found to be non-normally distributed and the number of samples is below 15 - use the Jackknife mean and UCL
Electrical Cable	Bootstrap Mean	1.49E+03	Standard Bootstrap UCL	2.56E+03	59	97%	29000	6.1	5	1	There is a sufficient number of values for statistical analysis - the data were found to be non-normal with high skewness, however, the Hall's transformed t bootstrap failed to normalize the dataset - use the Standard Bootstrap mean and UCL
Rubber Products	Bootstrap Mean	3.72E+01	Hall Adjusted Bootstrap	5.29E+01	30	83%	130	6.5	5	5	There is a sufficient number of values for statistical analysis - the data were found to be non-normally distributed with high skewness - use the Standard Bootstrap mean and Hall's Adjusted Bootstrap UCL
Vent Gaskets	Bootstrap Mean	2.05E+01	Standard Bootstrap UCL	3.14E+01	34	56%	210	5	1	1	There is a sufficient number of values for statistical analysis - the data were found to be non-normal with high skewness, however, the Hall's transformed t bootstrap failed to normalize the dataset - use the Standard Bootstrap mean and UCL

where:
UCL is 95% Upper Confidence Limit for the mean

Table 11

Mass Estimates of PCB-Containing Materials Onboard the ex-ORISKANY

PRAM Source Term	Corresponding CACI Source Term	Original Mass[1] (CACI Final Weight Report Mass) (lbs)	(kg)	Adjustment Factors A: CACI Source Term to PRAM Source Term Conversion	B: 30 Year Growth	C: Mass Remaining After Preparation	Current Material Mass (FWR Mass*A*B*C) (lbs)	(kg)	PCB Adj Factor: PCB Fraction in Material (%)	Current PCB Mass: Current Material Mass * Fraction PCB (lbs)	(kg)
Vent Gasket Material	Vent Gaskets	2,680	1,216	1	1.2	100%	3,216	1,459	0.00314	10.09824	4.58049006
Lubricants	Lubricants	208,140	94,411	1	1	0%	0	0	0.01	0	0
Foam Rubber Material	N/A	0	0	N/A	N/A	N/A	0	0	0.76	0	0
Black Rubber Material	Rubber Products	11,898	5,397	1	1	100%	11,898	5,397	0.0053	63.0594	28.6032967
Electrical Cable (insulation + wires)	Cable Insulation (insulation only)	403,600	183,070	1.384	1.3	90%	653,490	296,419	0.185	120895.682	54837.4243
Bulkhead Insulation Material	Bulkhead Insulation	115,695	52,478	1	1	27.4%	31,700	14,379	0.054	1711.82322	776.470875
Aluminum Paint	Paints	298,999	135,624	1	3	95%	852,147	386,528	0.002	1704.2943	773.05581

Notes:

Pape, L. Thomas. 2004. Final Report – Polychlorinated biphenyls (PCB) Source Term Estimates for ex-ORISKANY (CVA 34) Rev. 4. CACI International Inc.

FIGURES

Figure 1

Flow Diagram for the Development of an Environmental Fate and Transport Model (adapted from Mackay et al., 1995)

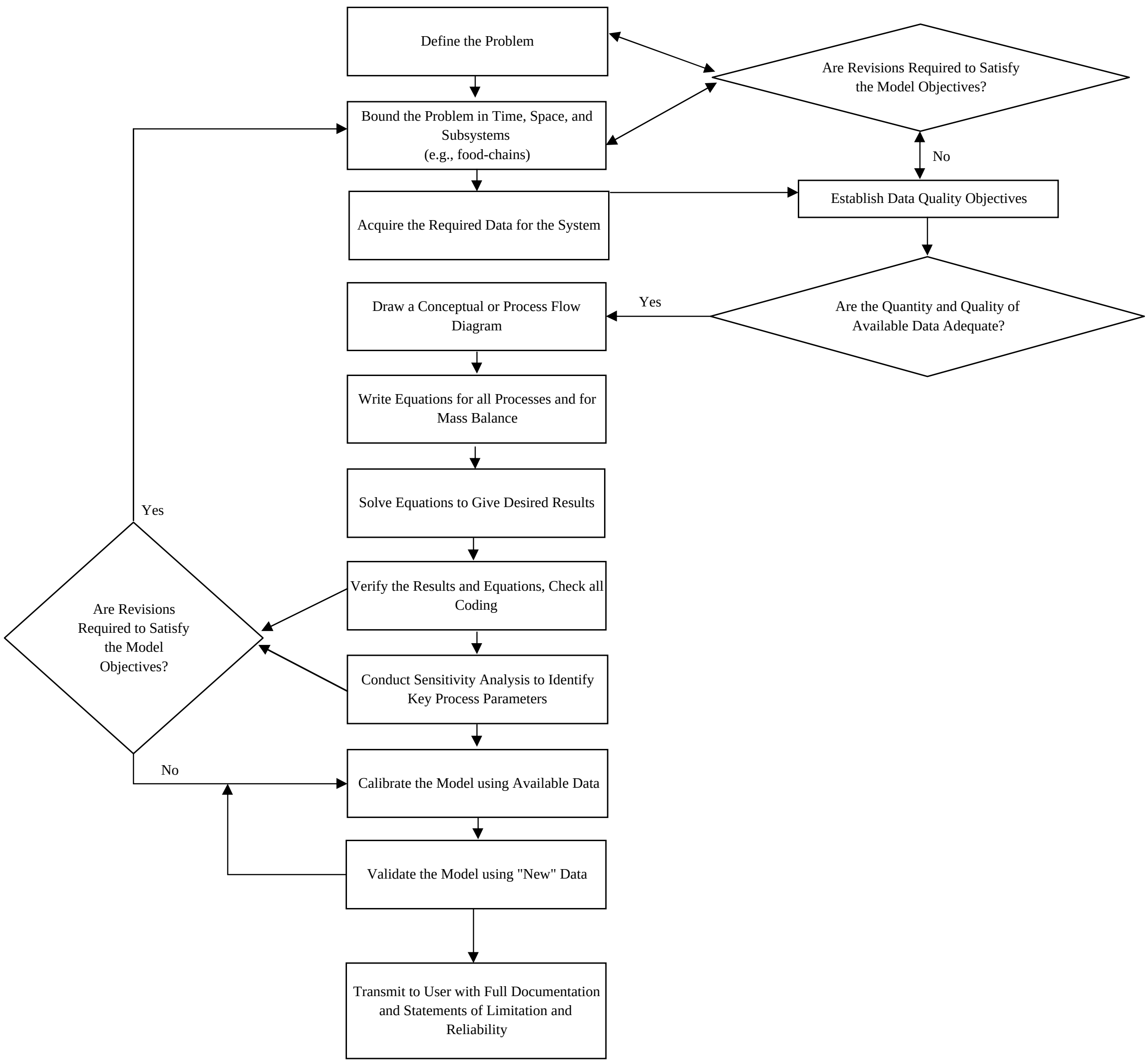


Figure 2

PRAM: Modules, Input, and Outputs

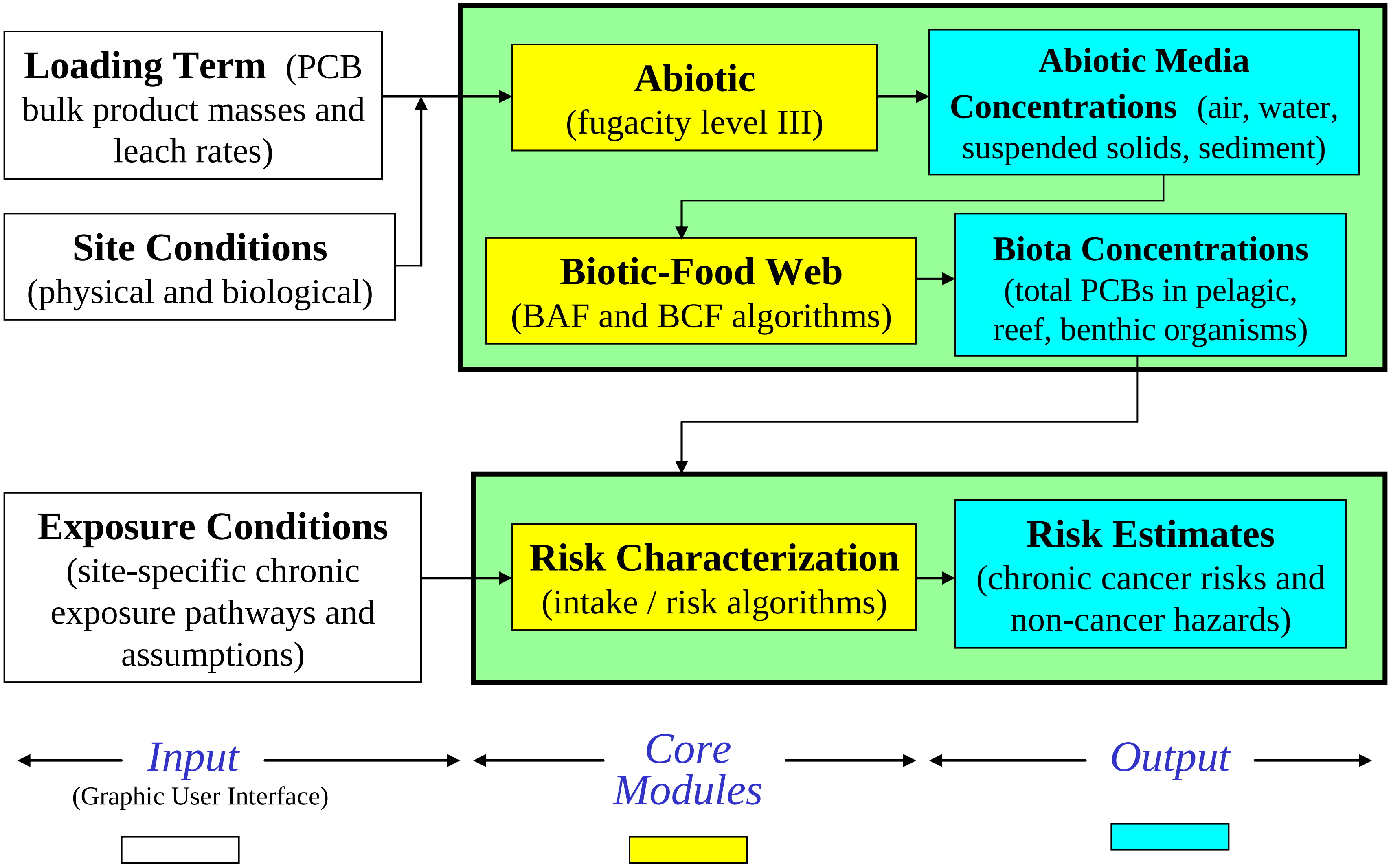


Figure 3

Abiotic and Biotic-Food Web Modules in PRAM

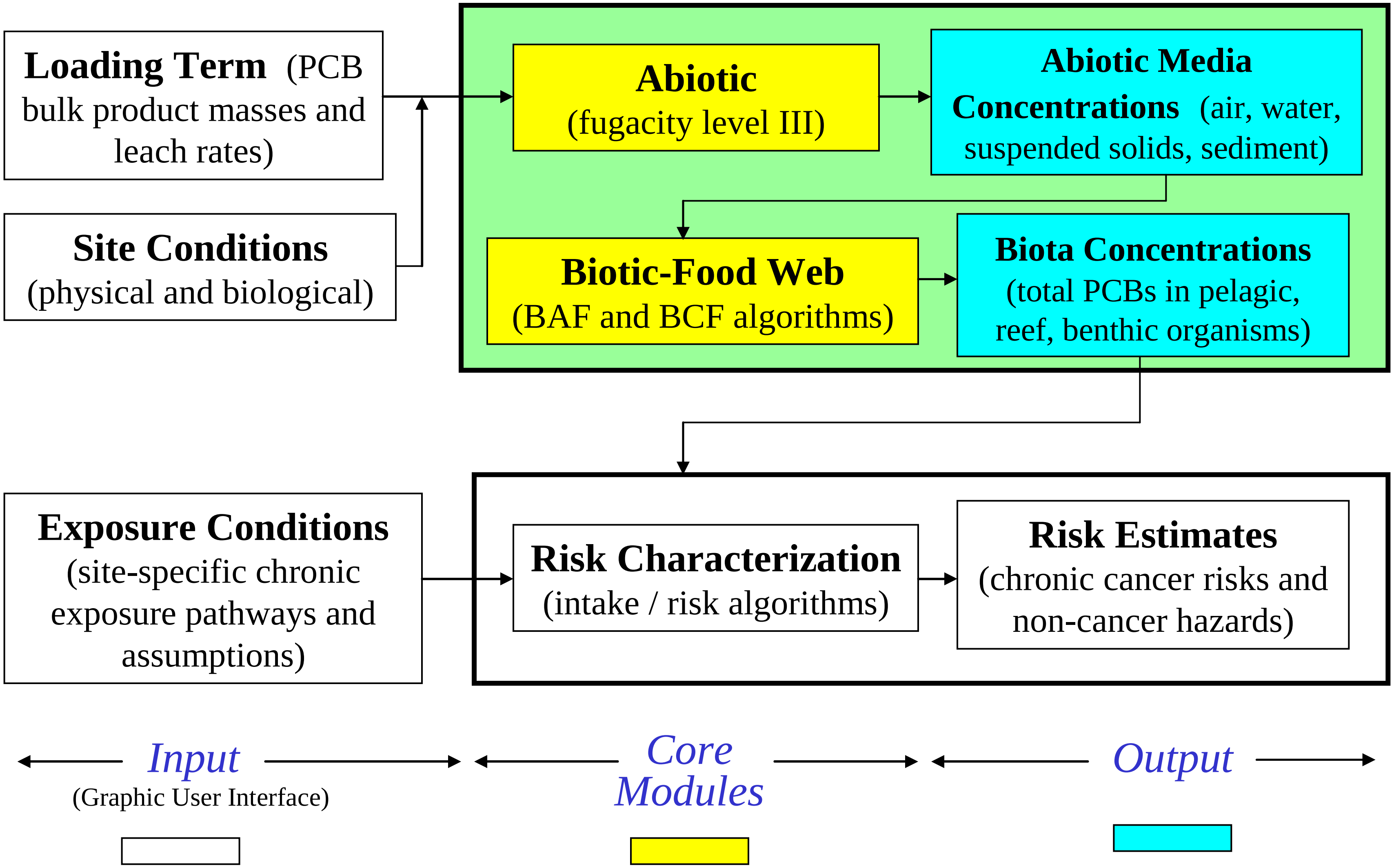
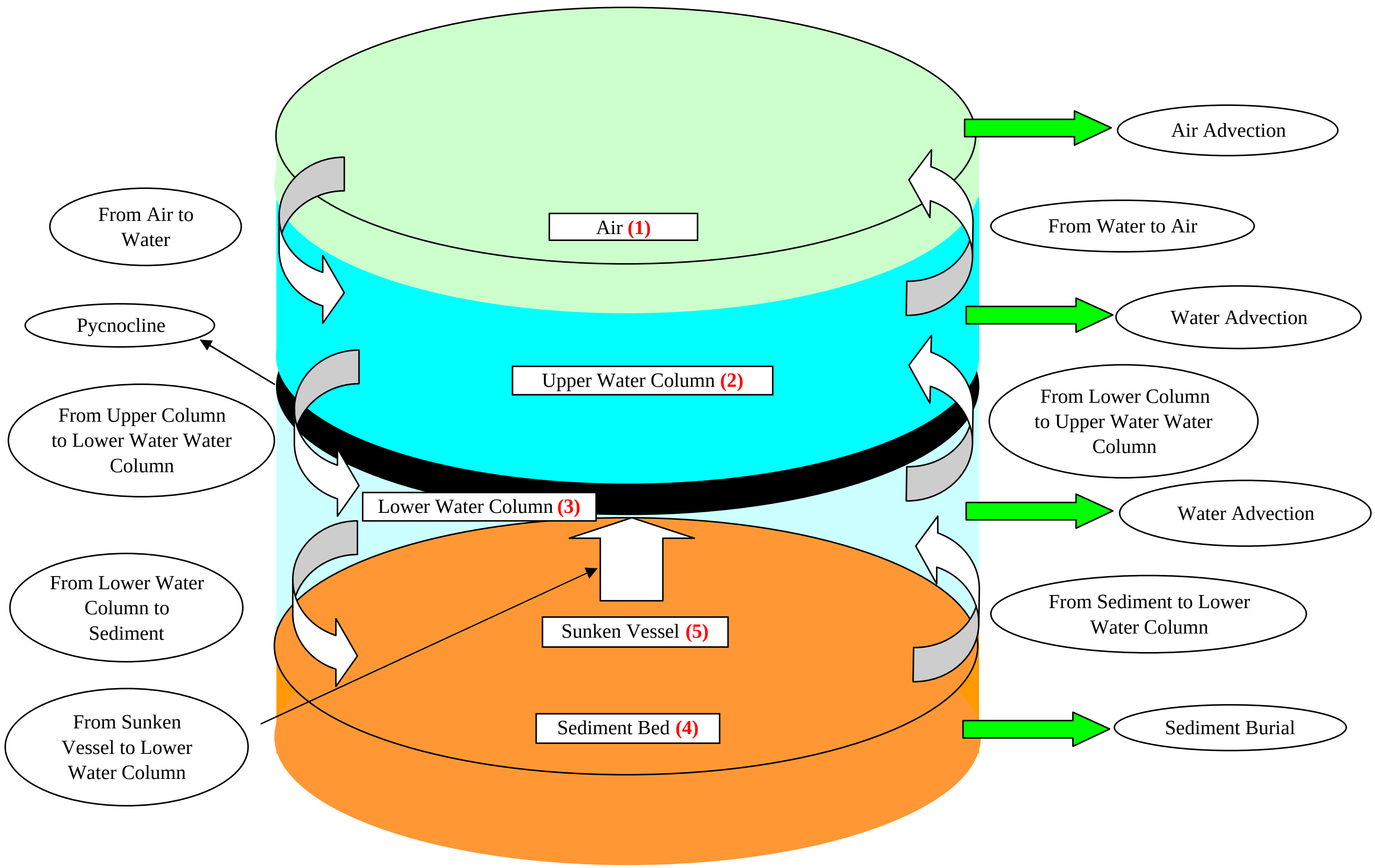


Figure 4

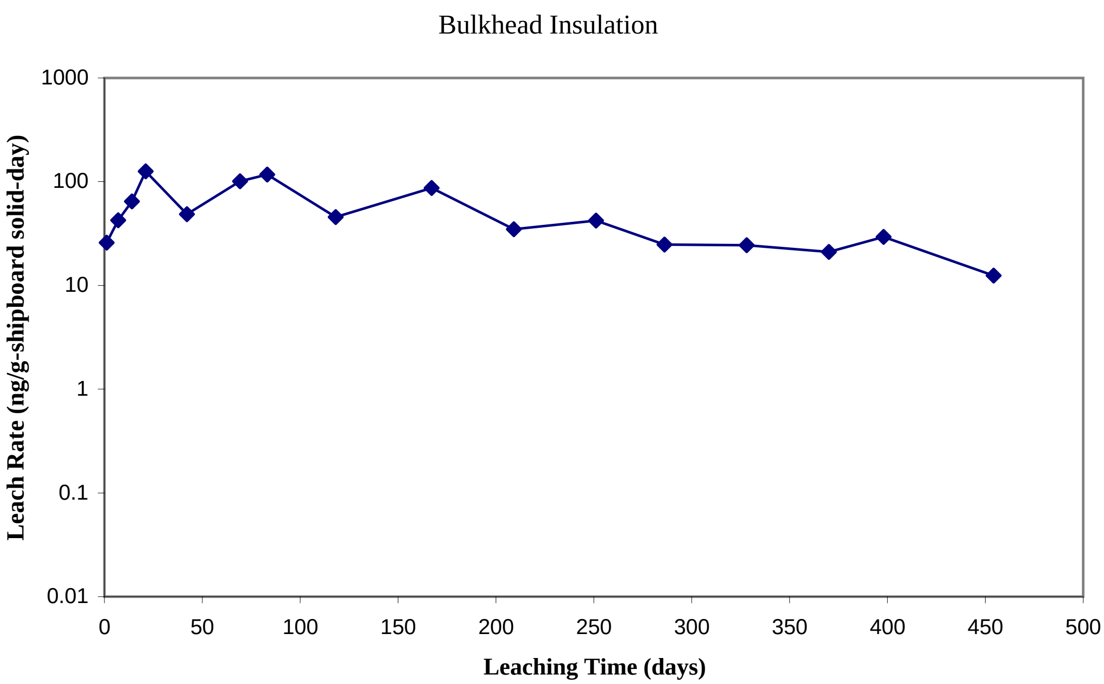
Compartment Identification for PCB Transport in PRAM



Reactive (Transformation) Processes are not presented

Figure 5

Example PCB Leach Rate Study Results:
Pentachlorobiphenyl (CL5) in Bulkhead Insulation and Ventilation Gaskets
(Adapted from R. George, SSC-SD, 2004)



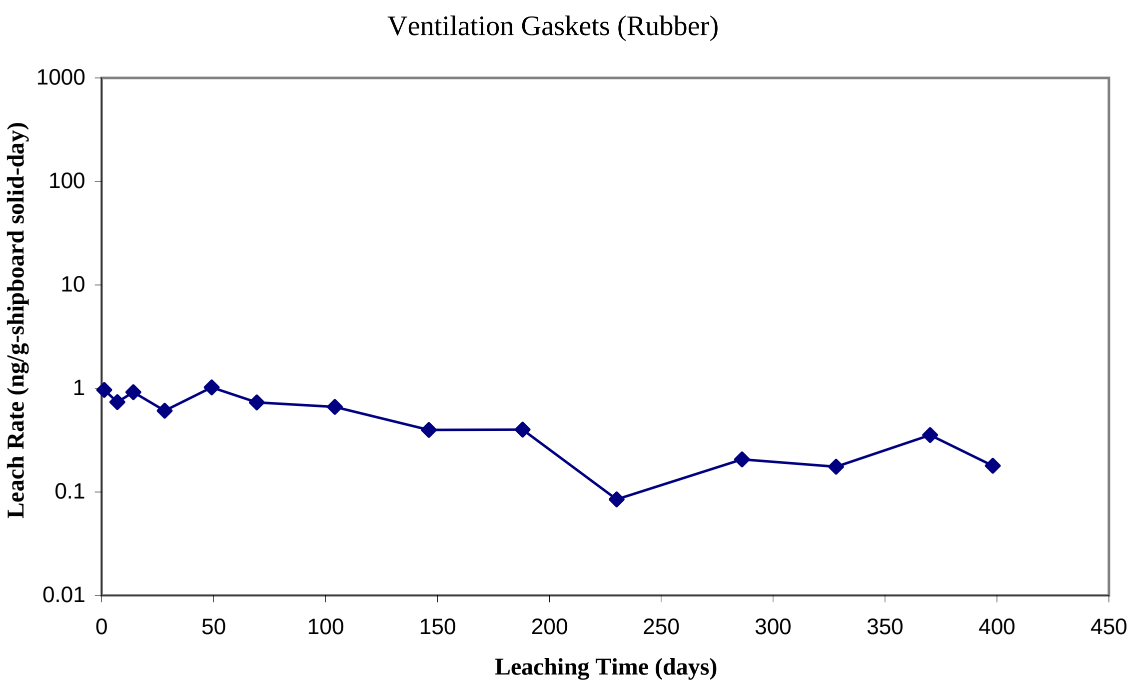
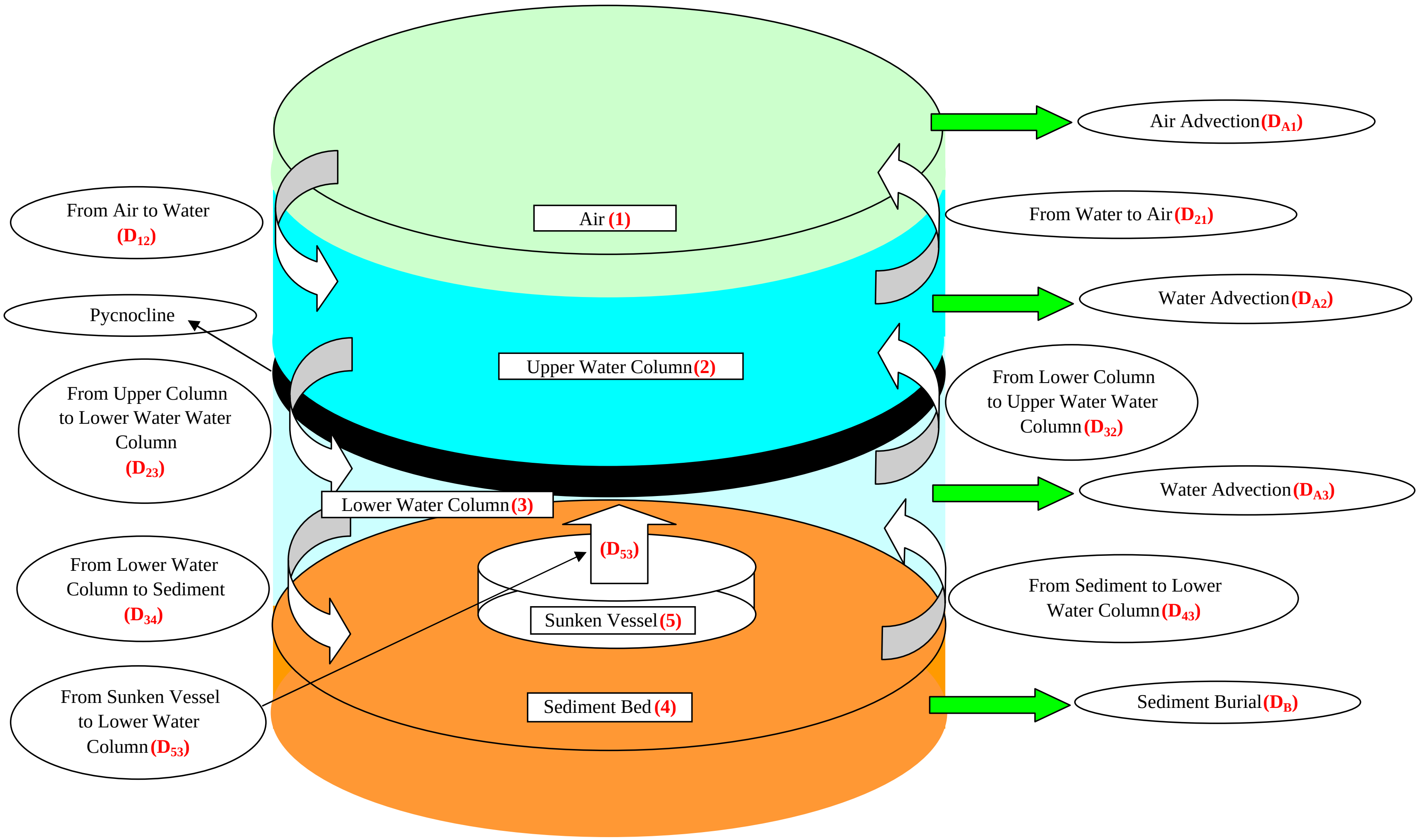


Figure 6

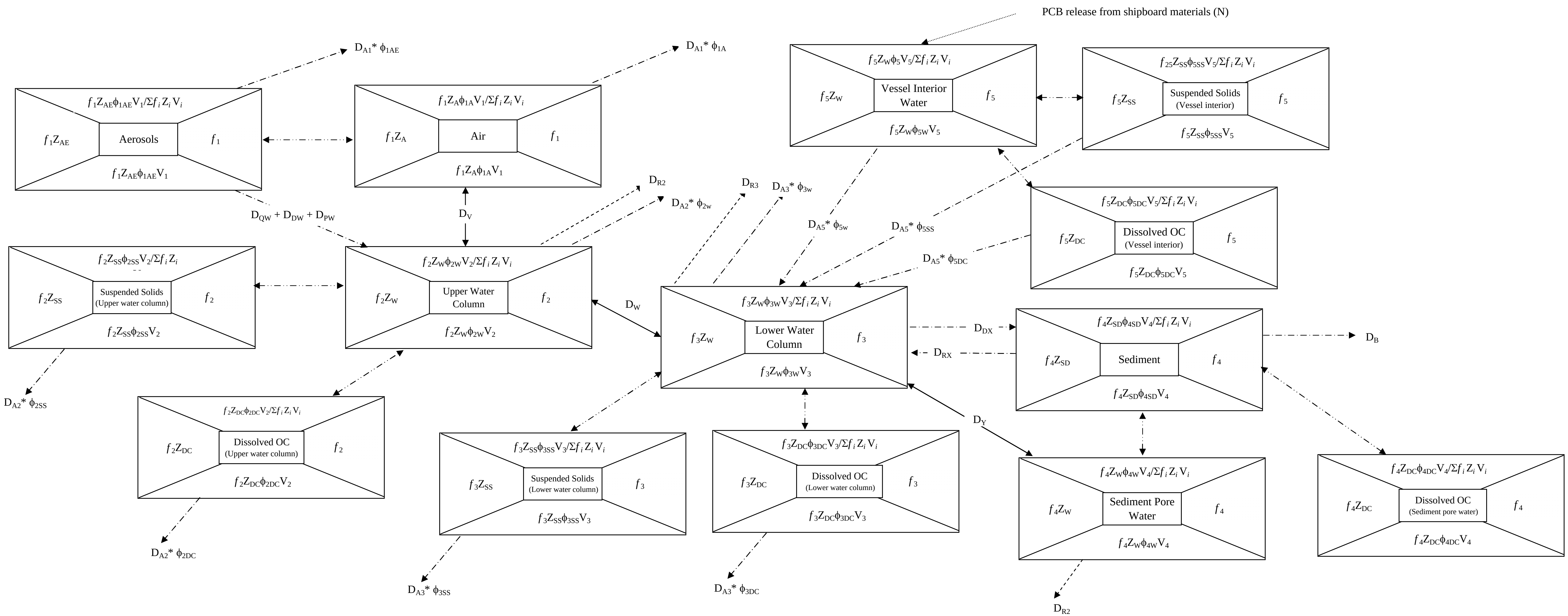
Transport Coefficients and Conceptual Design for PCB Transport in PRAM

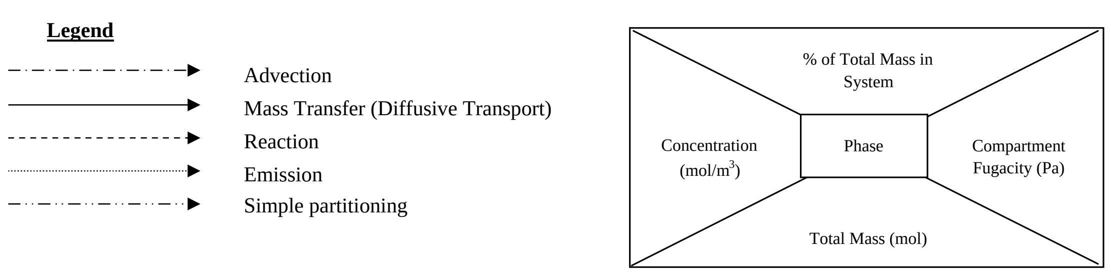


Reactive (Transformation) Processes are not presented

Figure 7

Fugacity-Based Transport and Transfers of PCBs in PRAM

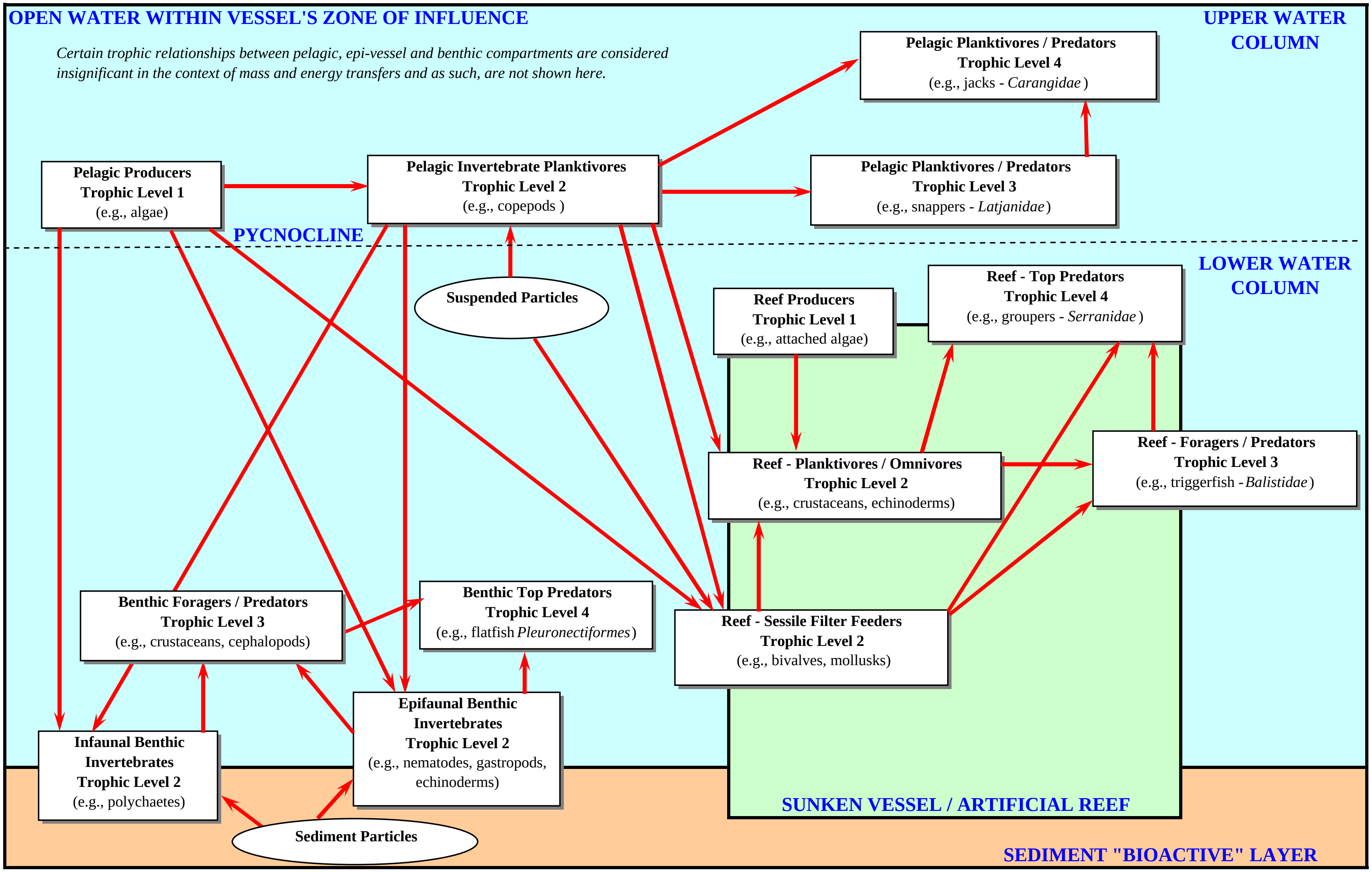




where:
f = fugacity
ϕ = volume fraction of specific media within compartment
Z = fugacity capacity of media (mol/m^3-Pa)
V = volume of compartment (m^3)
D_{ij} = fugacity mass transfer coefficient (mol/Pa-day)

Figure 8

Depiction of Food Web Used in PRAM

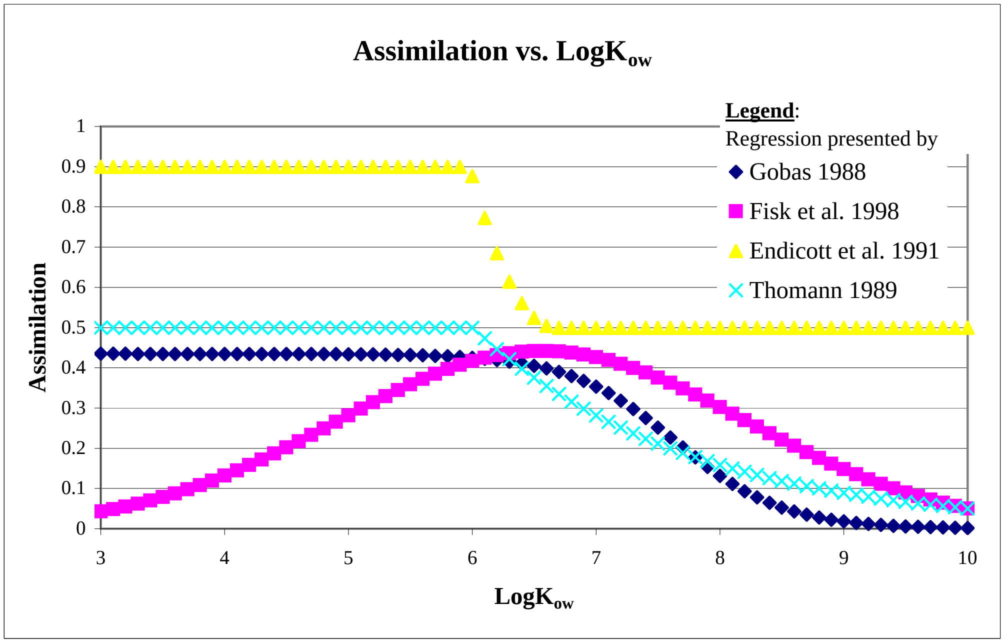


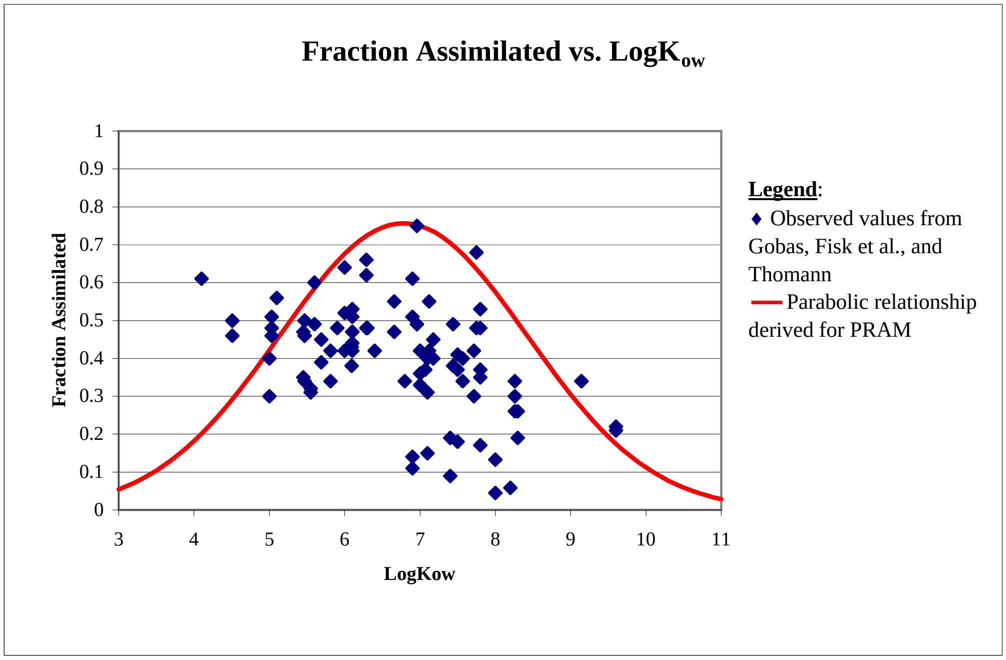
*Some organisms split their residence time between the Upper and Lower Water Columns.

Arrows indicate the direction for the flow of energy and mass

Figure 9

Assimilation Efficiencies Across Gastro-Intestinal Tracts as Function of Chemical-Specific K_{ow} in the Food Web Module of PRAM



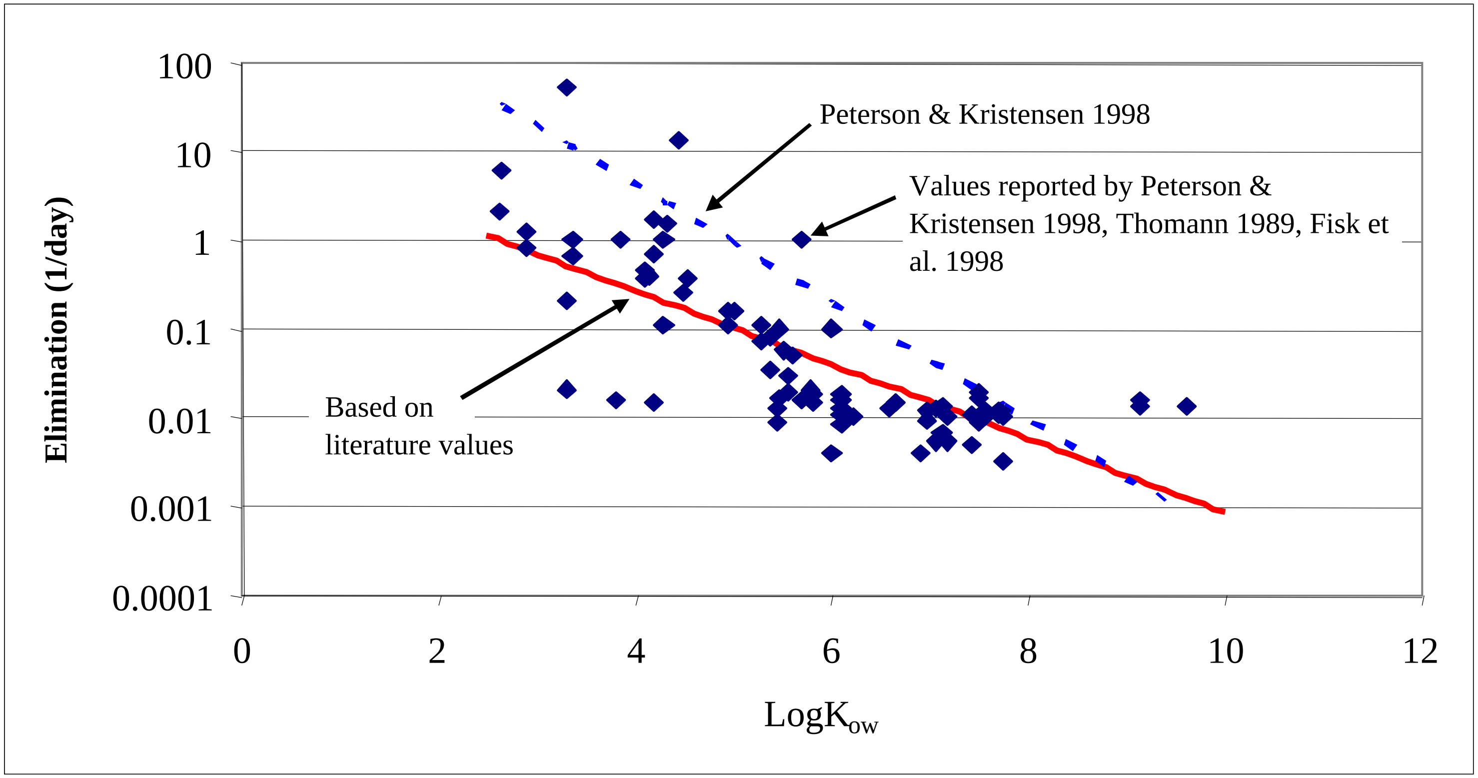


Review of the raw data suggested that the form of the relationship between K_{ow} and α is perhaps best described as a parabolic function. A parabolic function was calibrated to assure a level of conservatism within the PRAM such virtually all of the reported assimilation efficiencies fell below the predicted values. The resultant algorithm is presented below and graphically compared to the observed values reported by Gobas et al. (1988), Thomann (1989), and Fisk et al. (1998).

$$\alpha = \frac{10^{-1.8+1.08 \log Kow - 0.08 \log Kow^2}}{100}$$

Figure 10

Relationship Between K_{ow} and Elimination Rates (Ke) of PCB in Aquatic Animals



Based on Peterson & Kristensen (1998) data only

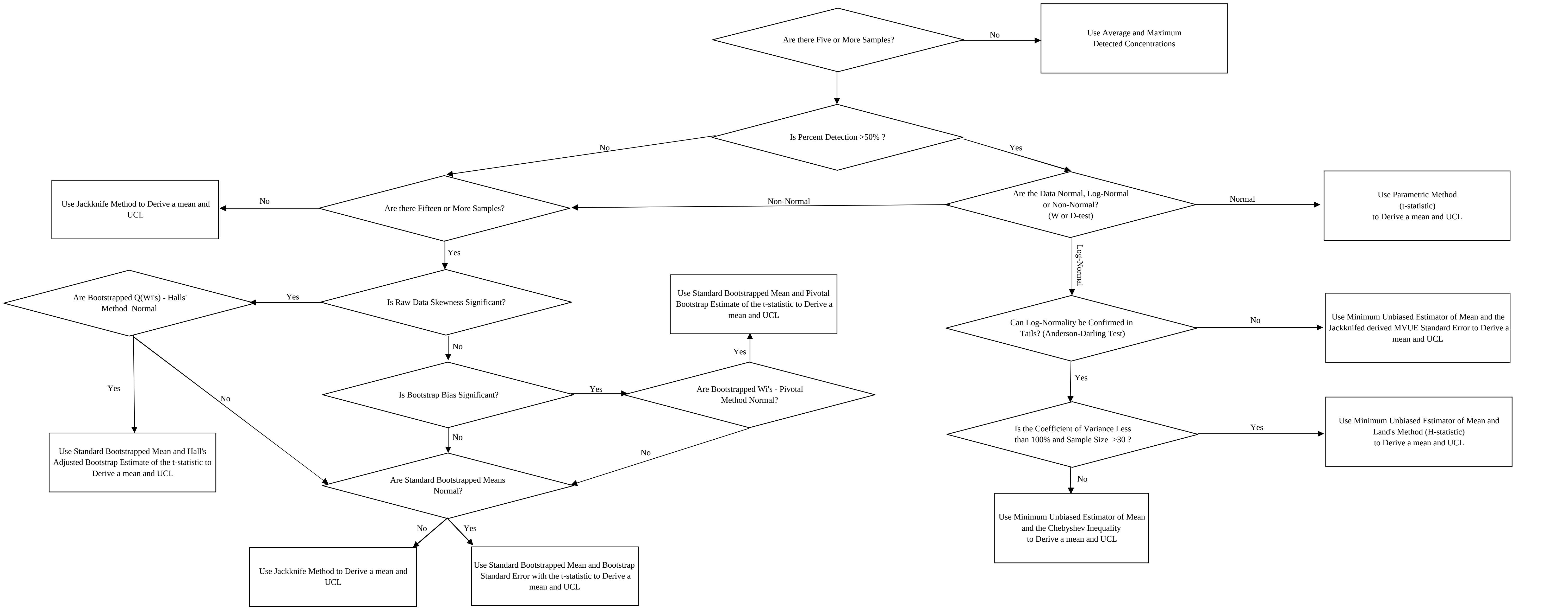
$$\log_{10} Ke\left[\frac{1}{day}\right] = 3.25 - 0.66 \times \log_{10} Kow$$

Based on literature values (used in the PRAM)

$$\log_{10} Ke\left[\frac{1}{day}\right] = 1.065 - 0.4131 \times \log_{10} Kow$$

Figure 11

Logic Diagram for Statistical Estimation of Reasonable Maximum PCB Concentration and Central Tendency Concentration in Source Material Onboard the Ex-ORISKANY

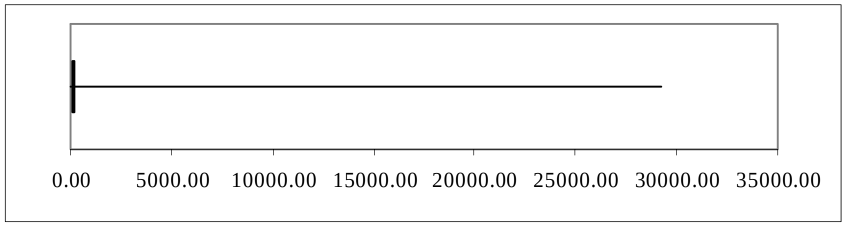


MVUE = minimum variance unbiased estimator
UCL = 95% upper confidence limit for the mean

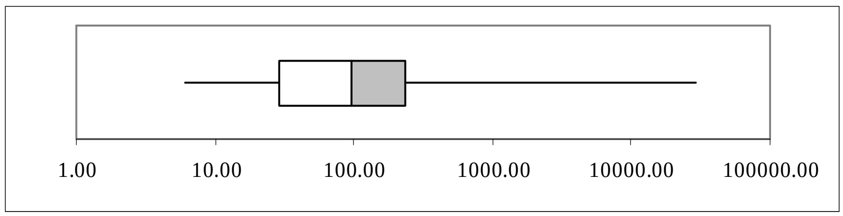
Figure 12

PCB Concentrations Presented as Box-Whisker Plots for Materials Found Onboard the Ex-ORSIKANY

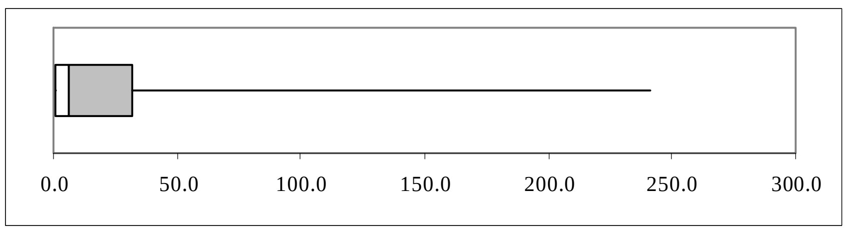
ELECTRICAL CABLE



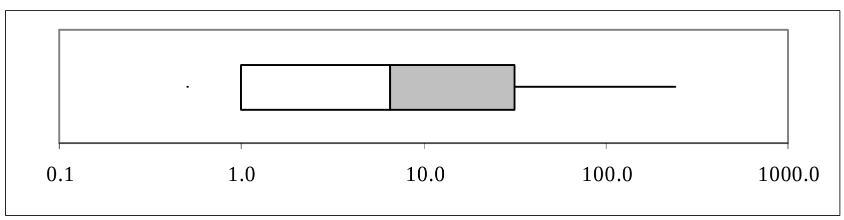
Quantiles for the data set	
Minimum	6.10
Lower Quartile	23.0
Median	67.0
Upper Quartile	140
Maximum	29000



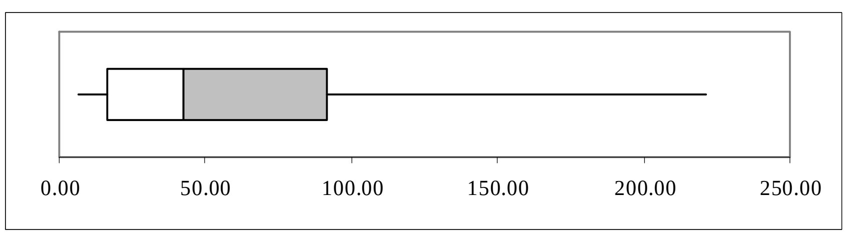
VENTILATION GASKETS



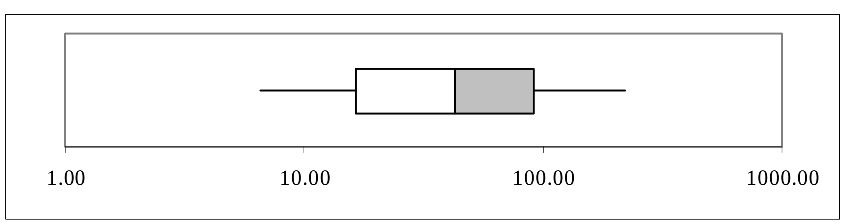
Quantiles for the data set	
Minimum	0.5
Lower Quartile	0.5
Median	5.5
Upper Quartile	25.0
Maximum	210



RUBBER MATERIALS



Quantiles for the data set	
Minimum	6.50
Lower Quartile	10.0
Median	26.0
Upper Quartile	49.0
Maximum	130

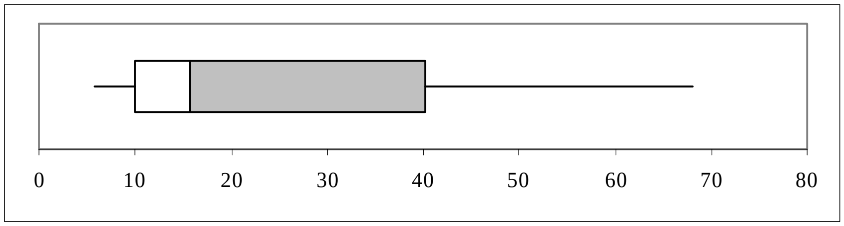


The lines represent min and max, white box = 25th to 50th quantile, gray box = 50th to 75th quantile, 50th = the median value

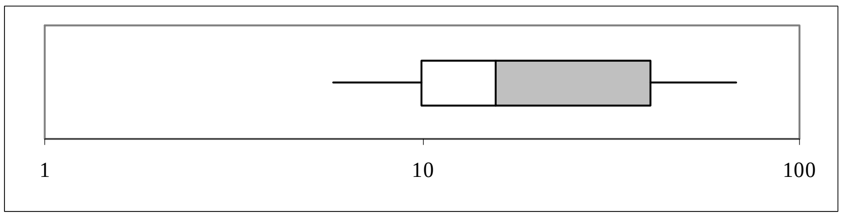
Figure 12

PCB Concentrations Presented as Box-Whisker Plots for Materials Found Onboard the Ex-ORSIKANY

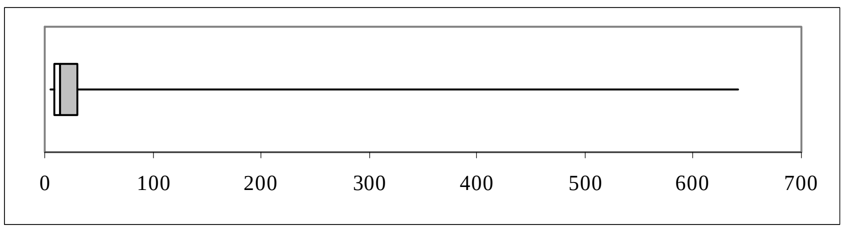
PAINTS



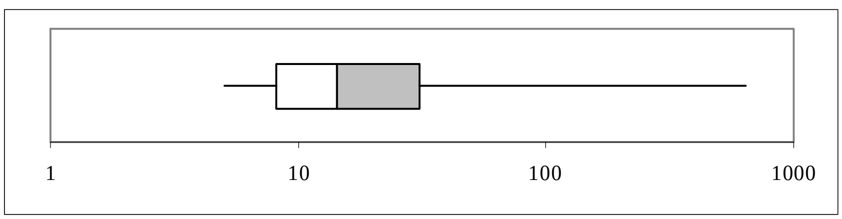
Quantiles for the data set	
Minimum	5.8
Lower Quartile	4.12
Median	5.8
Upper Quartile	24.4
Maximum	28



BULKHEAD INSULATION



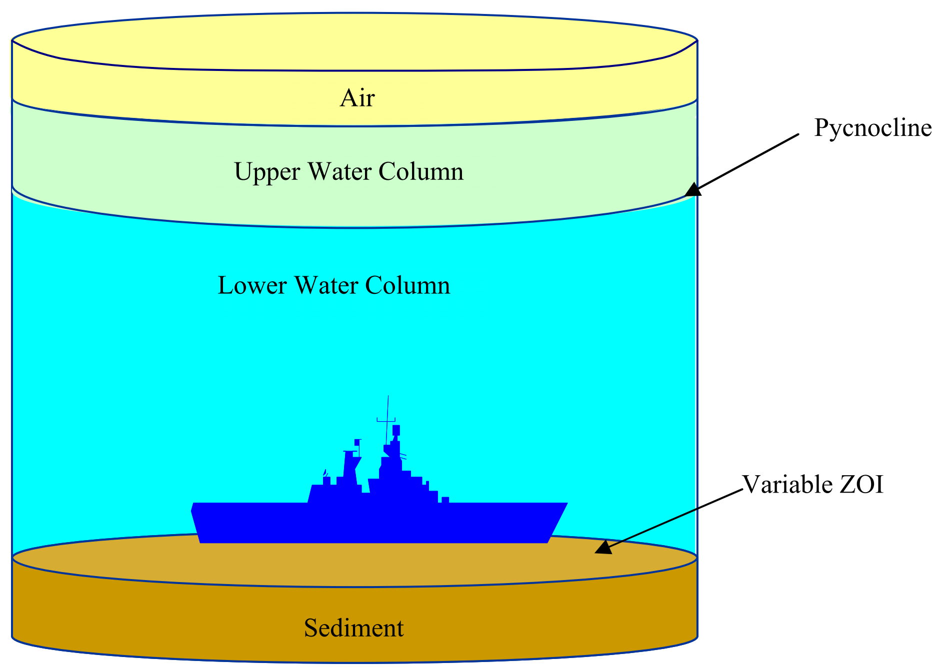
Quantiles for the data set	
Minimum	5
Lower Quartile	3.18
Median	6.15
Upper Quartile	16.5
Maximum	610



The lines represent min and max, white box = 25th to 50th quantile, gray box = 50th to 75th quantile, 50th = the median value

Figure 13

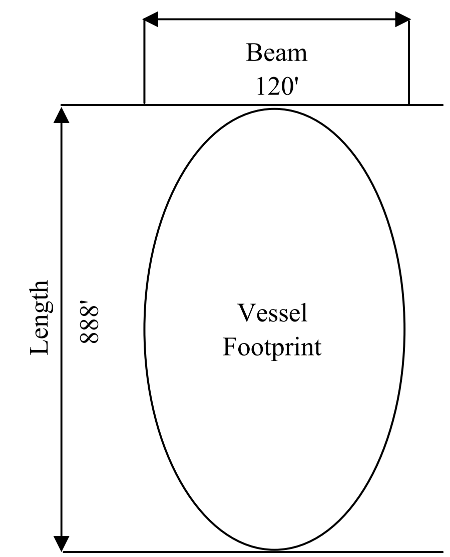
Zone of Influence (ZOI) Ellipse Area Calculations



SIDE VIEW

Zone of Influence determines spatial footprint on ocean floor. PRAM models this elliptical footprint through upper and lower water columns as well as air space above vessel.

ZOI = 1 is equivalent to vessel footprint



If ZOI = 1

Footprint = Vessel Footprint

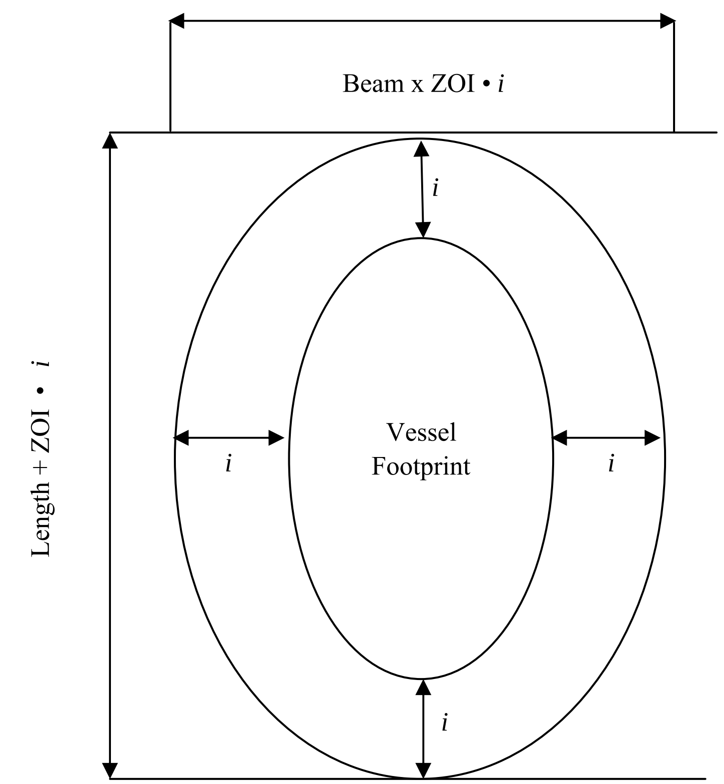
= Area of Ellipse

$$= \pi\left(\frac{\text{Length}}{2}\right)\left(\frac{\text{Beam}}{2}\right)$$

$$= \pi\left(\frac{888}{2}\right)\left(\frac{120}{2}\right)$$

$$= \pi(444)(60)$$

$$\approx 83{,}700\ \text{ft}^2$$



For ZOI >1

Solve for increment, *i*

$$\text{Vessel footprint} \bullet \text{ZOI} = \frac{\pi}{4}(\text{L} + 2i)(\text{W} + 2i)$$

$$\frac{\pi}{4}\text{LW ZOI} = \frac{\pi}{4}\left(\text{LW} + 2i\text{W} + 2i\text{L} + 4i^2\right)$$

$$4\text{i}^2 + 2\text{i}(\text{W} + \text{L}) + (1 - \text{ZOI})\text{LW} = 0$$

$$i^2 + \frac{i}{2}(\text{W} + \text{L}) - \frac{(\text{ZOI} - 1)\text{LW}}{4} = 0$$

Solve quadratic equation for *i*

Figure 14

Risk Characterization Module in PRAM

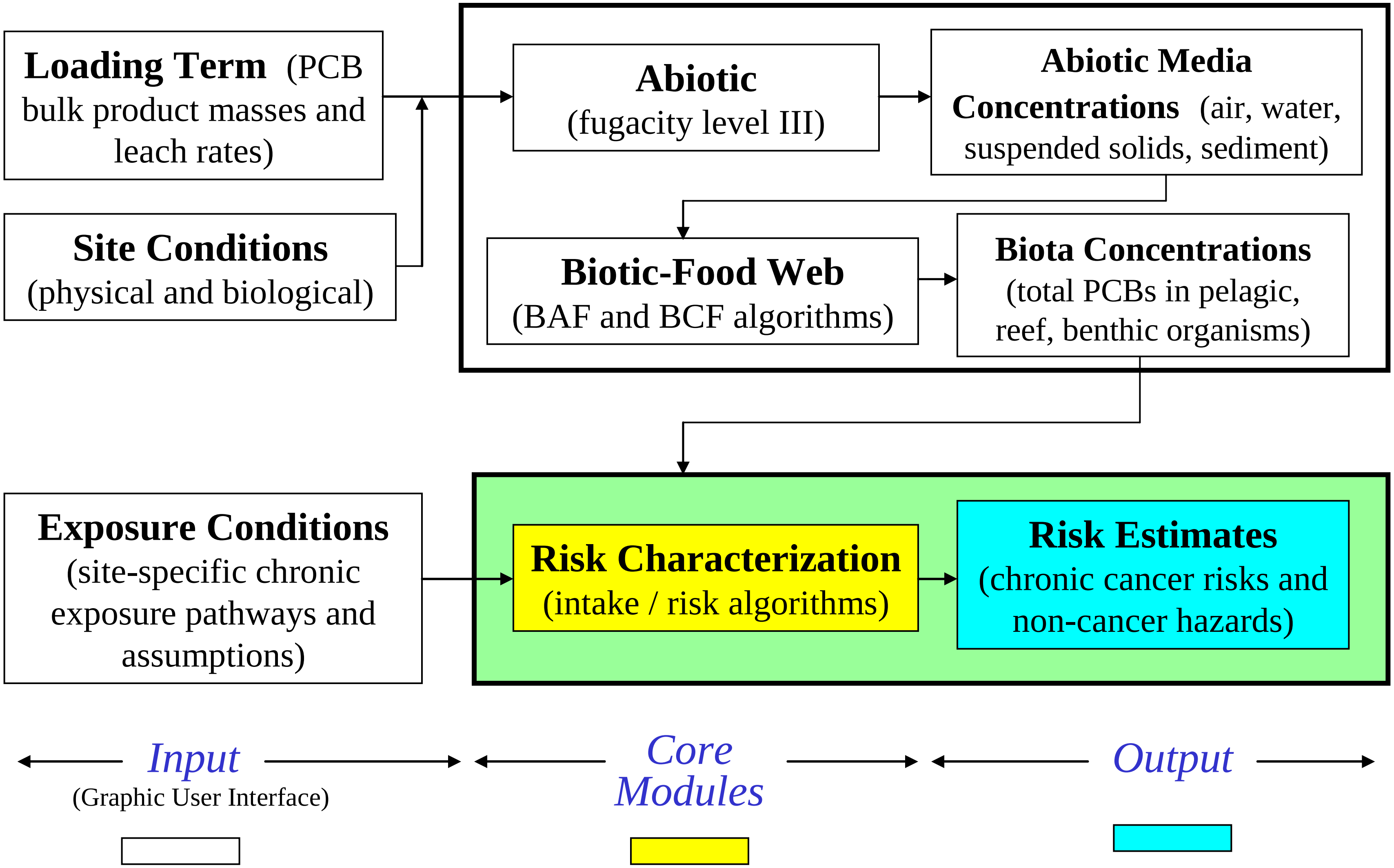
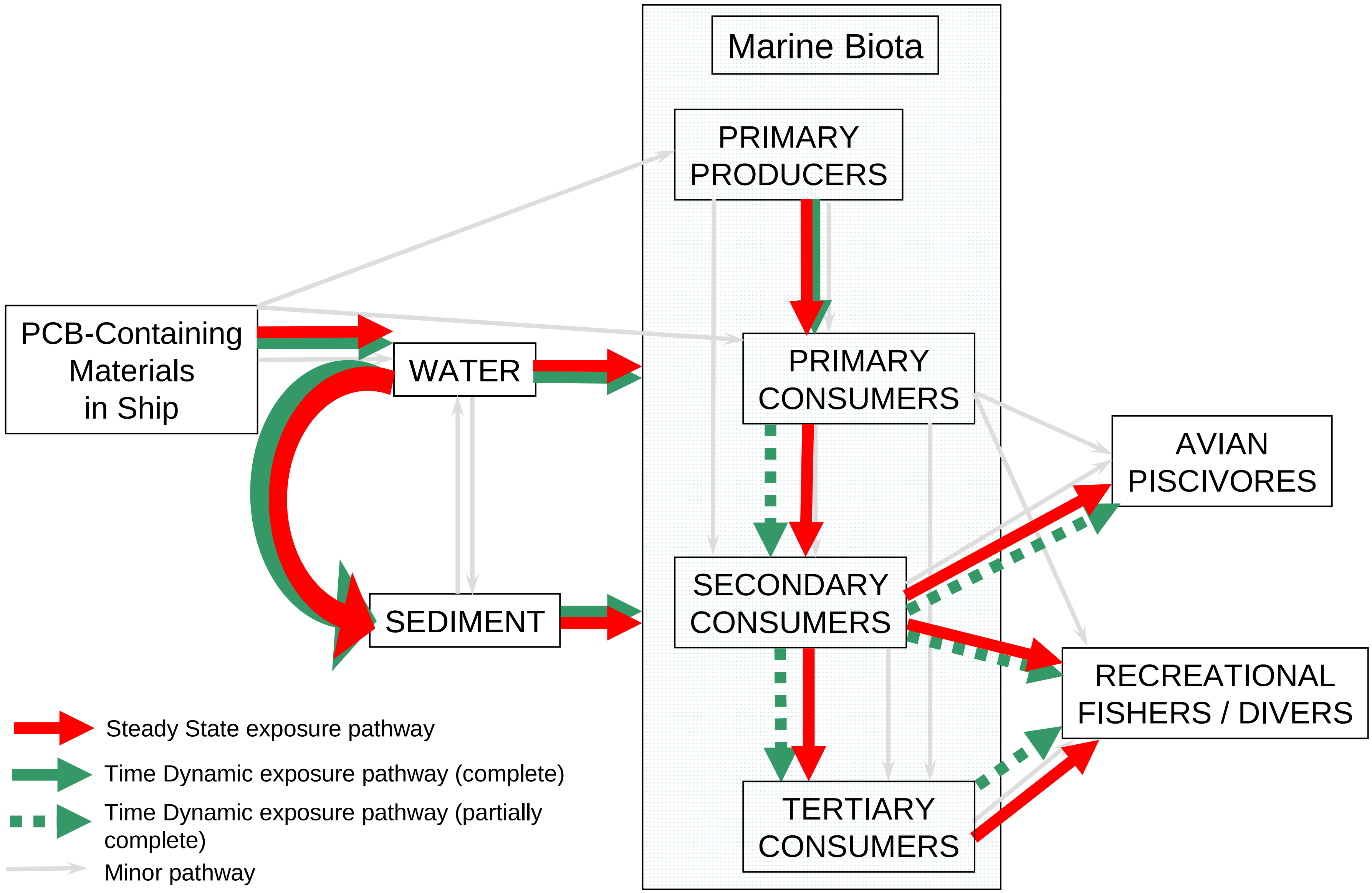


Figure 15

SCEM - Site Conceptual Exposure Model



APPENDIX A

REGRESSION ANALYSES: PCB LEACH RATES AND MATERIAL FRACTIONS

LEACH RATES

ALUMINIZED PAINT

Aluminized Paint

Leaching Time (days) ng/g material-d	**Homologue Leach Rates (ng PCB/g shipboard solid-day)** Cl1	Cl2	Cl3	Cl4	Cl5	Cl6	Cl7	Cl8	Cl9	Cl10
0.008	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
1.101	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	3.1E+00	0.0E+00	0.0E+00	0.0E+00
7.022	0.0E+00	0.0E+00	0.0E+00	5.0E-01	0.0E+00	0.0E+00	5.7E-01	0.0E+00	0.0E+00	0.0E+00
21.076	0.0E+00	0.0E+00	1.1E-01	4.4E-01	9.6E-01	4.8E-01	4.0E-01	0.0E+00	0.0E+00	0.0E+00
42.044	0.0E+00	0.0E+00	0.0E+00	1.3E-01	8.3E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
71.241	0.0E+00	0.0E+00	0.0E+00	1.2E-01	7.5E-01	5.7E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00
105.081	0.0E+00	0.0E+00	0.0E+00	1.4E-01	4.9E-01	3.6E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00
147.088	0.0E+00	0.0E+00	0.0E+00	2.4E-01	7.8E-01	5.1E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00
189.030	0.0E+00	0.0E+00	0.0E+00	2.0E-01	5.9E-01	3.4E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00
231.006	0.0E+00	0.0E+00	0.0E+00	1.2E-01	5.2E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
273.125	0.0E+00	0.0E+00	0.0E+00	4.2E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
315.042	0.0E+00	0.0E+00	0.0E+00	4.4E-02	2.9E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
357.008	0.0E+00	0.0E+00	0.0E+00	1.6E-01	6.7E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
399.022	0.0E+00	0.0E+00	0.0E+00	4.9E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
469.032	0.0E+00	0.0E+00	0.0E+00	6.2E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
Max	0.0E+00	0.0E+00	1.1E-01	5.0E-01	9.6E-01	5.7E-01	3.1E+00	0.0E+00	0.0E+00	0.0E+00
Min	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00

0.00043 g PCB / g paint (leachate study concentration)

Leaching Time (days) ng/ g-PCB - d	**Homologue Leach Rates (ng PCB/g PCB-day)** Cl1	Cl2	Cl3	Cl4	Cl5	Cl6	Cl7	Cl8	Cl9	Cl10
0.008	0	0	0	0	0	0	0	0	0	0
1.101	0	0	0	0	0	0	7191	0	0	0
7.022	0	0	0	1165	0	0	1314	0	0	0
21.076	0	0	261	1021	2240	1108	921	0	0	0
42.044	0	0	0	300	1919	0	0	0	0	0
71.241	0	0	0	272	1739	1333	0	0	0	0
105.081	0	0	0	324	1150	836	0	0	0	0
147.088	0	0	0	547	1810	1179	0	0	0	0
189.030	0	0	0	459	1376	793	0	0	0	0
231.006	0	0	0	283	1209	0	0	0	0	0
273.125	0	0	0	97	0	0	0	0	0	0
315.042	0	0	0	101	68	0	0	0	0	0
357.008	0	0	0	383	1559	0	0	0	0	0
399.022	0	0	0	114	0	0	0	0	0	0
469.032	0	0	0	144	0	0	0	0	0	0
Max	0	0	261	1165	2240	1333	7191	0	0	0
Min	0	0	0	0	0	0	0	0	0	0
Median	0	0	0	283	1150	0	0	0	0	0
Simple Average	0	0	17.4	347	871	350	628	0	0	0
Detects	0	0	1	13	10	5	3	0	0	0
Non-detects	15	15	14	2	5	10	12	15	15	15
Intercept	---	---	---	8.09E+00	9.74E+00	8.69E+00	8.85E+00	---	---	---
Slope	---	---	---	-4.96E-01	-5.70E-01	-3.69E-01	-7.19E-01	---	---	---
alpha	---	---	---	1.92E-03	1.67E-01	3.88E-01	1.37E-01	---	---	---

Tetrachlorobiphenyl in Aluminized Paint

ng/ g-PCB - d	C14
7.64E-03	0
1.10E+00	0
7.02E+00	1165
2.11E+01	1021
4.20E+01	300
7.12E+01	272
1.05E+02	324
1.47E+02	547
1.89E+02	459
2.31E+02	283
2.73E+02	97
3.15E+02	101
3.57E+02	383
3.99E+02	114
4.69E+02	144

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
1.95E+00	7.02E+00	1165	7.06E+00
3.05E+00	2.11E+01	1021	6.93E+00
3.74E+00	4.20E+01	300	5.70E+00
4.27E+00	7.12E+01	272	5.61E+00
4.65E+00	1.05E+02	324	5.78E+00
4.99E+00	1.47E+02	547	6.30E+00
5.24E+00	1.89E+02	459	6.13E+00
5.44E+00	2.31E+02	283	5.65E+00
5.61E+00	2.73E+02	97	4.57E+00
5.75E+00	3.15E+02	101	4.62E+00
5.88E+00	3.57E+02	383	5.95E+00
5.99E+00	3.99E+02	114	4.73E+00
6.15E+00	4.69E+02	144	4.97E+00

Maximum Release Rate at 7 day
1165 ng/gPCB-d

Release rate at 2 years
123.3 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.7736
R Square	0.5985
Standard Error	0.5371
Observations	13

ANOVA

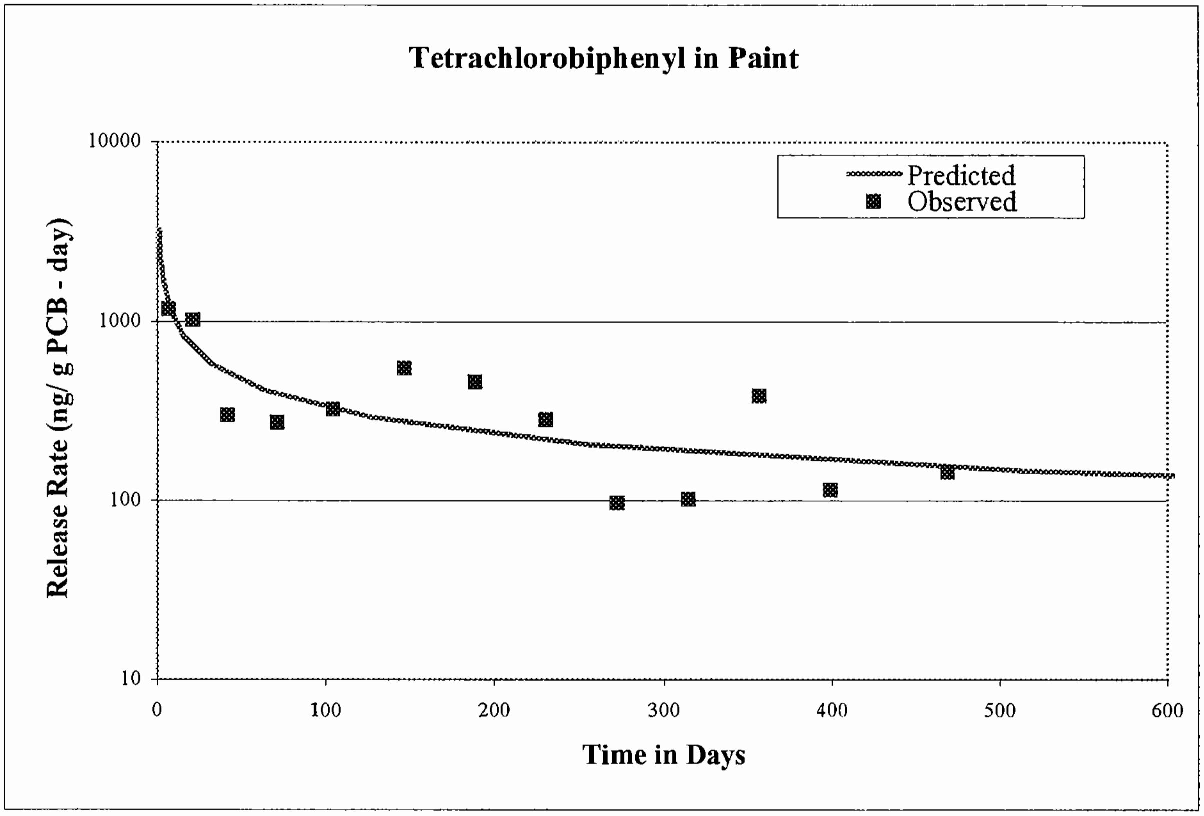
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	4.73E+00	4.73E+00	1.64E+01	1.92E-03
Residual	11	3.17E+00	2.88E-01		
Total	12	7.90E+00			

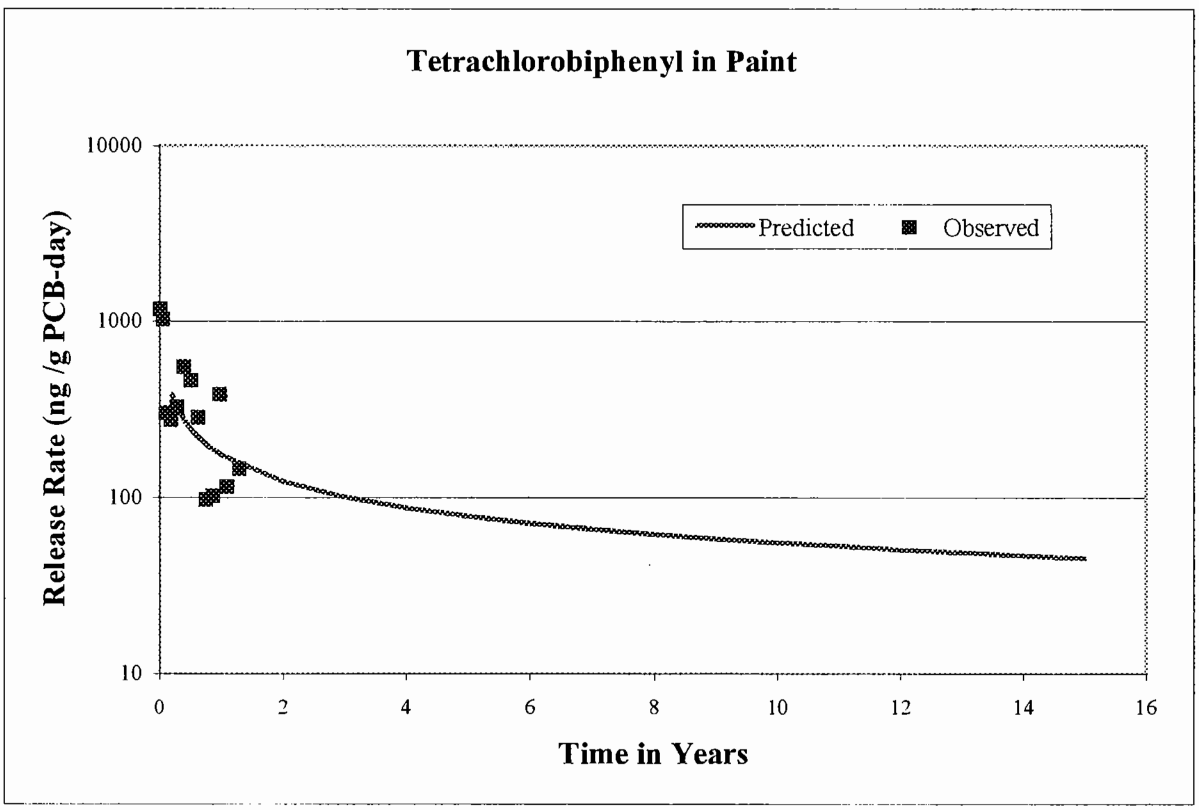
	Coefficients	*andard Errc*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	8.09E+00	6.09E-01	1.33E+01	4.11E-08	6.74E+00	9.43E+00
ln(day)	-4.96E-01	1.22E-01	-4.05E+00	1.92E-03	-7.66E-01	-2.26E-01

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	7.12E+00	-5.81E-02
2	6.57E+00	3.55E-01
3	6.23E+00	-5.26E-01
4	5.97E+00	-3.62E-01
5	5.78E+00	4.31E-03
6	5.61E+00	6.95E-01
7	5.49E+00	6.43E-01
8	5.39E+00	2.61E-01
9	5.30E+00	-7.32E-01
10	5.23E+00	-6.14E-01
11	5.17E+00	7.79E-01
12	5.11E+00	-3.82E-01

13	5.03E+00	-6.48E-02





Pentachlorobiphenyl in Aluminized Paint

ng/ g-PCB - d	Cl5
7.64E-03	0
1.10E+00	0
7.02E+00	0
2.11E+01	2240
4.20E+01	1919
7.12E+01	1739
1.05E+02	1150
1.47E+02	1810
1.89E+02	1376
2.31E+02	1209
2.73E+02	0
3.15E+02	68
3.57E+02	1559
3.99E+02	0
4.69E+02	0

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
3.05E+00	2.11E+01	2240	7.71E+00
3.74E+00	4.20E+01	1919	7.56E+00
4.27E+00	7.12E+01	1739	7.46E+00
4.65E+00	1.05E+02	1150	7.05E+00
4.99E+00	1.47E+02	1810	7.50E+00
5.24E+00	1.89E+02	1376	7.23E+00
5.44E+00	2.31E+02	1209	7.10E+00
5.75E+00	3.15E+02	68	4.21E+00
5.88E+00	3.57E+02	1559	7.35E+00

Maximum Release Rate at 21 day
2240 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.5038
R Square	0.2538
Standard Error	0.9926
Observations	9

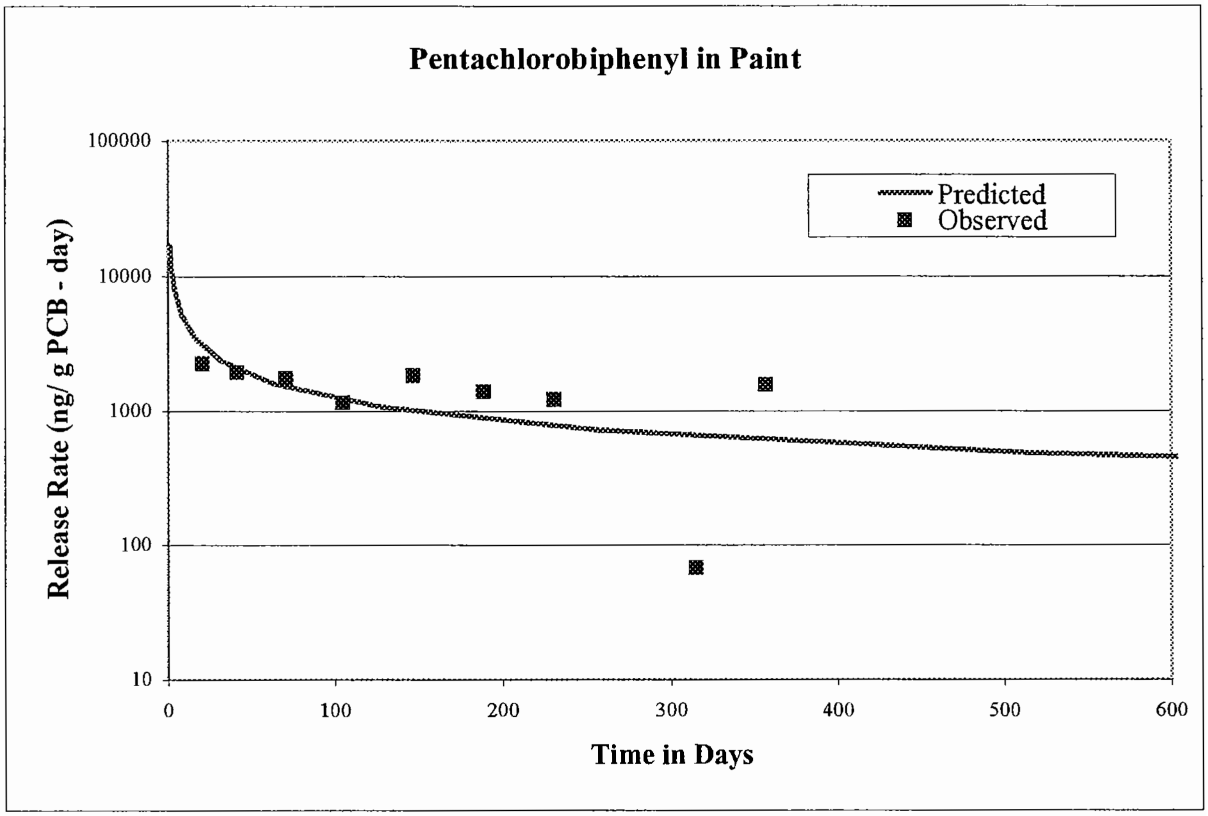
ANOVA

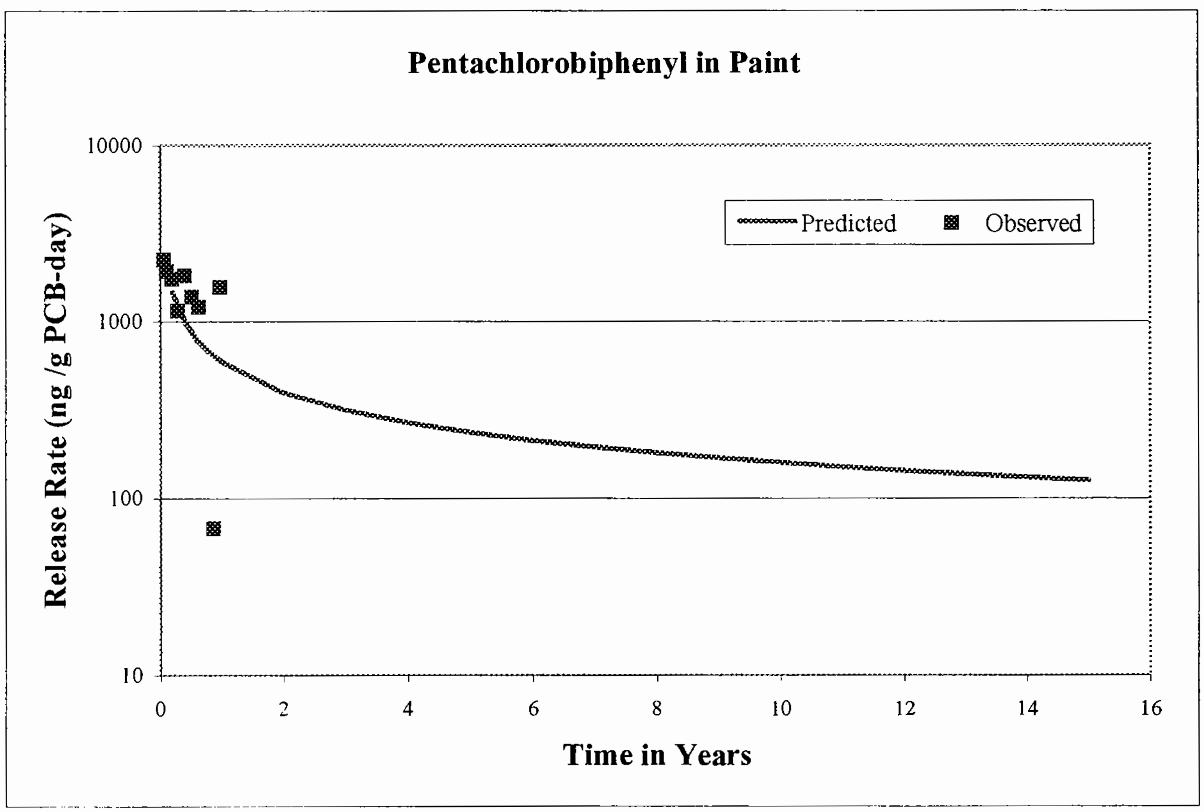
	df	*SS*	*MS*	*F*	*Significance F*	
Regression	1	2.35E+00	2.35E+00	2.38E+00	1.67E-01	***Not Significant***
Residual	7	6.90E+00	9.85E-01			
Total	8	9.24E+00				

	Coefficients	*andard Errc*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	9.74E+00	1.80E+00	5.42E+00	9.85E-04	5.49E+00	1.40E+01
ln(day)	-5.70E-01	3.70E-01	-1.54E+00	1.67E-01	-1.44E+00	3.04E-01

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	8.01E+00	-2.92E-01
2	7.61E+00	-5.31E-02
3	7.31E+00	1.49E-01
4	7.09E+00	-4.29E-02
5	6.90E+00	6.03E-01
6	6.76E+00	4.72E-01
7	6.64E+00	4.56E-01
8	6.46E+00	-2.25E+00
9	6.39E+00	9.59E-01


Pentachlorobiphenyl in Paint
Predicted
Observed
100000
10000
1000
100
10
Release Rate (ng/ g PCB - day)
0
100
200
300
400
500
600
Time in Days


Pentachlorobiphenyl in Paint
Predicted
Observed
10000
1000
100
10
Release Rate (ng /g PCB-day)
0
2
4
6
8
10
12
14
16
Time in Years

Hexachlorobiphenyl in Aluminized Paint

ng/ g-PCB - d	Cl6
7.64E-03	0
1.10E+00	0
7.02E+00	0
2.11E+01	1108
4.20E+01	0
7.12E+01	1333
1.05E+02	836
1.47E+02	1179
1.89E+02	793
2.31E+02	0
2.73E+02	0
3.15E+02	0
3.57E+02	0
3.99E+02	0
4.69E+02	0

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
4.27E+00	7.12E+01	1333	7.20E+00
4.65E+00	1.05E+02	836	6.73E+00
4.99E+00	1.47E+02	1179	7.07E+00
5.24E+00	1.89E+02	793	6.68E+00

Maximum Release Rate at 71 days
1333 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.6123
R Square	0.3749
Standard Error	0.2472
Observations	4

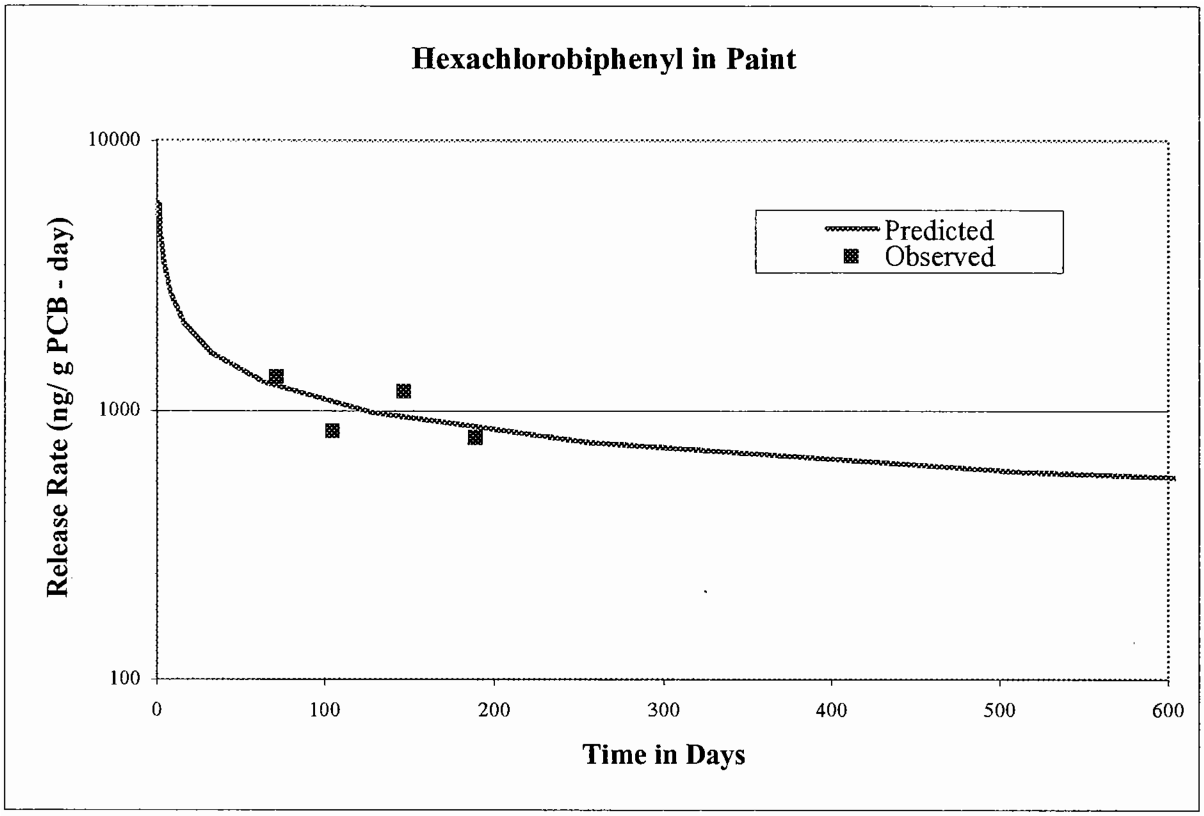
ANOVA

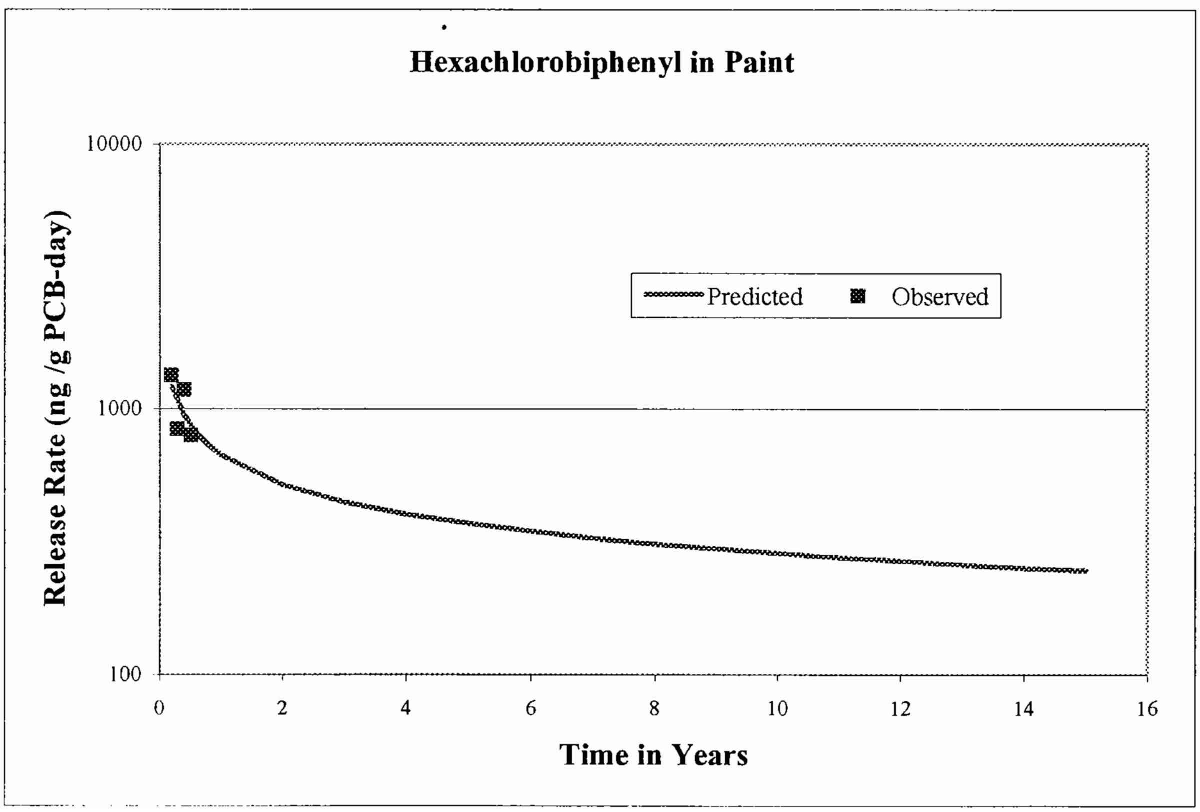
	df	*SS*	*MS*	*F*	*Significance F*	
Regression	1	7.33E-02	7.33E-02	1.20E+00	3.88E-01	***Not Significant***
Residual	2	1.22E-01	6.11E-02			
Total	3	1.95E-01				

	Coefficients	*andard Erro*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	8.69E+00	1.62E+00	5.36E+00	3.30E-02	1.72E+00	1.57E+01
ln(day)	-3.69E-01	3.37E-01	-1.10E+00	3.88E-01	-1.82E+00	1.08E+00

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	7.11E+00	8.46E-02
2	6.97E+00	-2.38E-01
3	6.84E+00	2.29E-01
4	6.75E+00	-7.53E-02


Hexachlorobiphenyl in Paint
Predicted
Observed
Release Rate (ng/ g PCB - day)
10000
1000
100
0
100
200
300
400
500
600
Time in Days


Hexachlorobiphenyl in Paint
Predicted
Observed
Release Rate (ng /g PCB-day)
10000
1000
100
0
2
4
6
8
10
12
14
16
Time in Years

Heptachlorobiphenyl in Aluminized Paint

ng/ g-PCB - d	Cl7
7.64E-03	0
1.10E+00	7191
7.02E+00	1314
2.11E+01	921
4.20E+01	0
7.12E+01	0
1.05E+02	0
1.47E+02	0
1.89E+02	0
2.31E+02	0
2.73E+02	0
3.15E+02	0
3.57E+02	0
3.99E+02	0
4.69E+02	0

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
9.66E-02	1.10E+00	7191	8.88E+00
1.95E+00	7.02E+00	1314	7.18E+00
3.05E+00	2.11E+01	921	6.83E+00

Maximum Release Rate at 1 day
7191 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.97703275
R Square	0.954592995
Standard Error	0.330974678
Observations	3

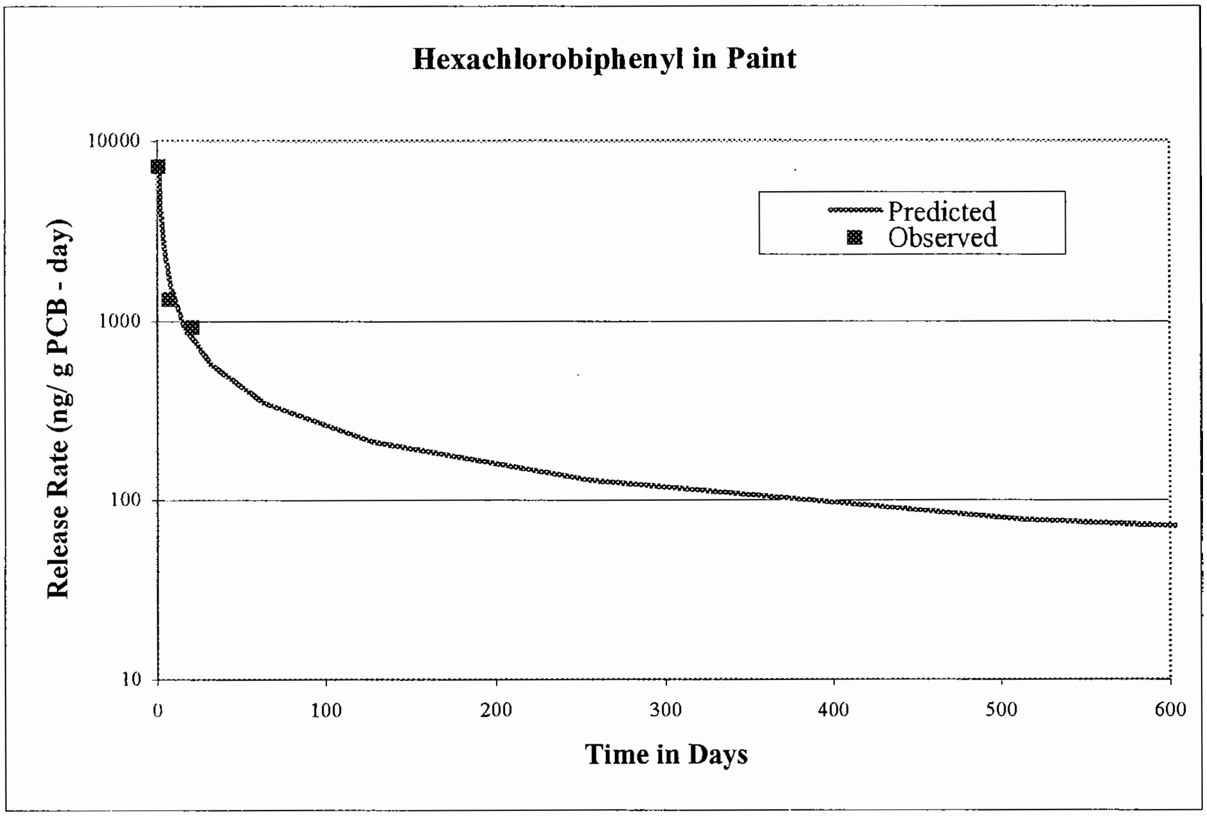
ANOVA

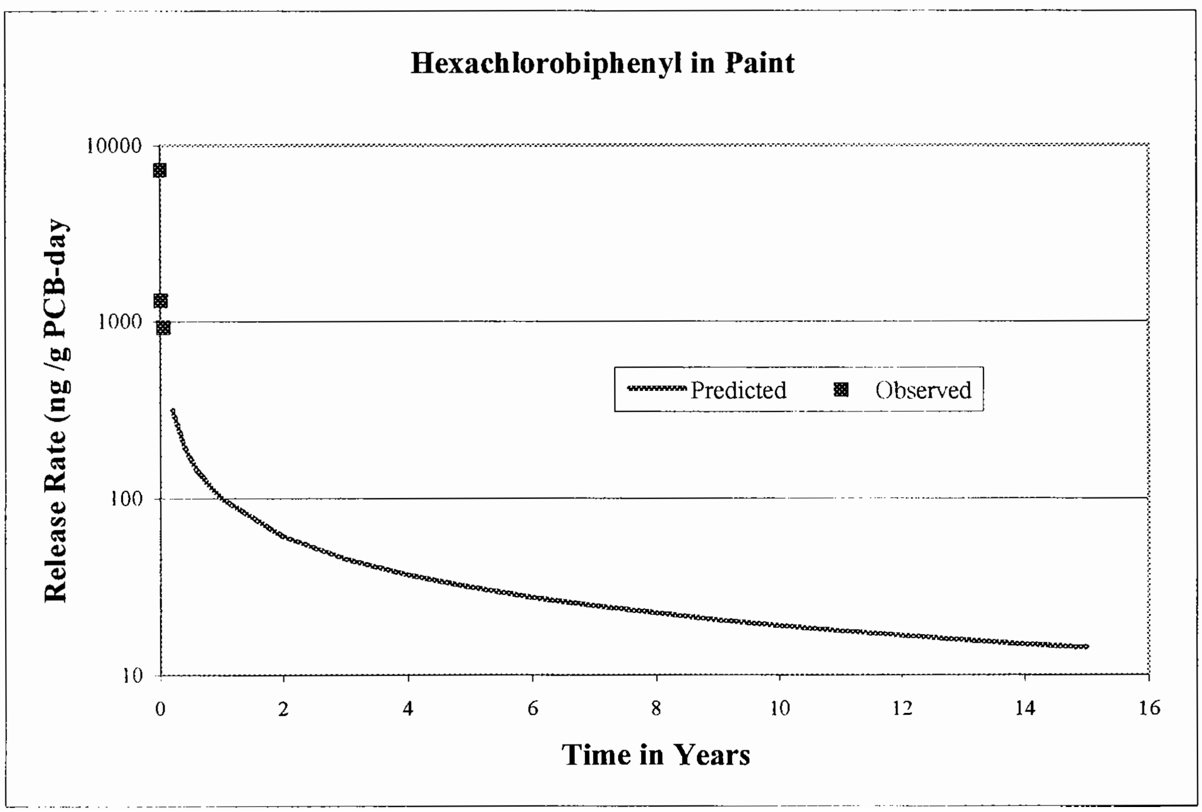
	df	*SS*	*MS*	*F*	*Significance F*	
Regression	1	2.30E+00	2.30E+00	2.10E+01	1.37E-01	***Not Significant***
Residual	1	1.10E-01	1.10E-01			
Total	2	2.41E+00				

	Coefficients	*andard Erro*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	8.85E+00	3.28E-01	2.70E+01	2.36E-02	4.68E+00	1.30E+01
ln(day)	-7.19E-01	1.57E-01	-4.59E+00	1.37E-01	-2.71E+00	1.27E+00

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	8.78E+00	9.96E-02
2	7.45E+00	-2.67E-01
3	6.66E+00	1.68E-01


Hexachlorobiphenyl in Paint
Release Rate (ng/ g PCB - day)
10000
1000
100
10
0
100
200
300
400
500
600
Time in Days
Predicted
Observed


Hexachlorobiphenyl in Paint
Release Rate (ng /g PCB-day
10000
1000
100
10
0
2
4
6
8
10
12
14
16
Time in Years
Predicted
Observed

AROCLOR 1254

Aroclor 1254

Leaching Time (days)	**Homologue Leach Rates (ng PCB/g shipboard solid-day)**									
	Cl1	Cl2	Cl3	Cl4	Cl5	Cl6	Cl7	Cl8	Cl9	Cl10
2.08E-03	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
1.03E+00	5.5E+02	1.6E+03	5.1E+02	1.3E+03	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
6.06E+00	4.6E+02	1.2E+03	8.5E+02	5.4E+03	1.1E+03	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
2.13E+01	2.9E+02	8.8E+02	7.0E+02	6.7E+03	2.8E+03	8.8E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00
4.23E+01	2.0E+02	6.4E+02	5.6E+02	7.6E+03	5.0E+03	3.2E+02	0.0E+00	0.0E+00	0.0E+00	0.0E+00
6.21E+01	2.1E+02	6.5E+02	6.2E+02	8.5E+03	6.9E+03	5.3E+02	0.0E+00	0.0E+00	0.0E+00	0.0E+00
6.93E+01	2.1E+02	8.0E+02	1.1E+03	2.3E+04	2.6E+04	2.6E+03	0.0E+00	0.0E+00	0.0E+00	0.0E+00
1.11E+02	8.6E+01	3.4E+02	3.4E+02	5.7E+03	5.3E+03	6.8E+02	0.0E+00	0.0E+00	0.0E+00	0.0E+00
1.46E+02	8.3E+01	3.4E+02	3.5E+02	6.0E+03	5.2E+03	5.5E+02	0.0E+00	0.0E+00	0.0E+00	0.0E+00
1.88E+02	6.6E+01	2.6E+02	2.7E+02	3.4E+03	3.0E+03	4.0E+02	0.0E+00	0.0E+00	0.0E+00	0.0E+00
2.30E+02	5.4E+01	2.5E+02	3.0E+02	6.1E+03	8.6E+03	1.2E+03	7.2E+01	0.0E+00	0.0E+00	0.0E+00
2.86E+02	5.2E+01	2.0E+02	1.7E+02	2.5E+03	2.1E+03	3.7E+02	0.0E+00	0.0E+00	0.0E+00	0.0E+00
3.31E+02	6.0E+01	2.8E+02	2.5E+02	3.2E+03	2.4E+03	3.5E+02	0.0E+00	0.0E+00	0.0E+00	0.0E+00
3.70E+02	3.1E+01	1.9E+02	1.9E+02	2.6E+03	1.6E+03	1.6E+02	0.0E+00	0.0E+00	0.0E+00	0.0E+00
4.33E+02	2.7E+01	1.4E+02	1.3E+02	1.9E+03	1.2E+03	1.4E+02	0.0E+00	0.0E+00	0.0E+00	0.0E+00
Max	5.5E+02	1.6E+03	1.1E+03	2.3E+04	2.6E+04	2.6E+03	7.2E+01	0.0E+00	0.0E+00	0.0E+00
Min	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
Median	8.3E+01	3.4E+02	3.4E+02	5.4E+03	2.8E+03	3.5E+02	0.0E+00	0.0E+00	0.0E+00	0.0E+00
Simple Average	1.6E+02	5.2E+02	4.2E+02	5.6E+03	4.8E+03	5.0E+02	4.8E+00	0.0E+00	0.0E+00	0.0E+00
Number of detects	14	14	14	14	13	12	1	0	0	0
Number of nondetects	1	1	1	1	2	3	14	15	15	15
intercept	6.96E+00	7.80E+00	1.05E+01	1.44E+01	1.57E+01	1.31E+01	---	---	---	---
slope	-5.17E-01	-4.02E-01	-9.18E-01	-1.12E+00	-1.40E+00	-1.30E+00	---	---	---	---
alpha	1.97E-06	1.70E-06	5.02E-04	7.49E-04	1.57E-03	4.18E-03	---	---	---	---

Monochlorobiphenyl in Aroclor 1254

ng/ g-PCB - d	Cl1
2.08E-03	0
1.03E+00	554
6.06E+00	459
2.13E+01	292
4.23E+01	197
6.21E+01	207
6.93E+01	215
1.11E+02	85.5
1.46E+02	83.2
1.88E+02	66.1
2.30E+02	54.0
2.86E+02	51.9
3.31E+02	60.5
3.70E+02	31.2
4.33E+02	27.2

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
2.54E-02	1.03E+00	554	6.32E+00
1.80E+00	6.06E+00	459	6.13E+00
3.06E+00	2.13E+01	292	5.68E+00
3.74E+00	4.23E+01	197	5.28E+00
4.13E+00	6.21E+01	207	5.33E+00
4.24E+00	6.93E+01	215	5.37E+00
4.71E+00	1.11E+02	86	4.45E+00
4.98E+00	1.46E+02	83	4.42E+00
5.24E+00	1.88E+02	66	4.19E+00
5.44E+00	2.30E+02	54	3.99E+00
5.66E+00	2.86E+02	52	3.95E+00
5.80E+00	3.31E+02	60	4.10E+00
5.91E+00	3.70E+02	31	3.44E+00
6.07E+00	4.33E+02	27	3.30E+00

Maximum Release Rate at 1 day
554 ng/gPCB-d

Release rate at 2 years
34.7 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.9263
R Square	0.8581
Standard Error	0.3793
Observations	14

ANOVA

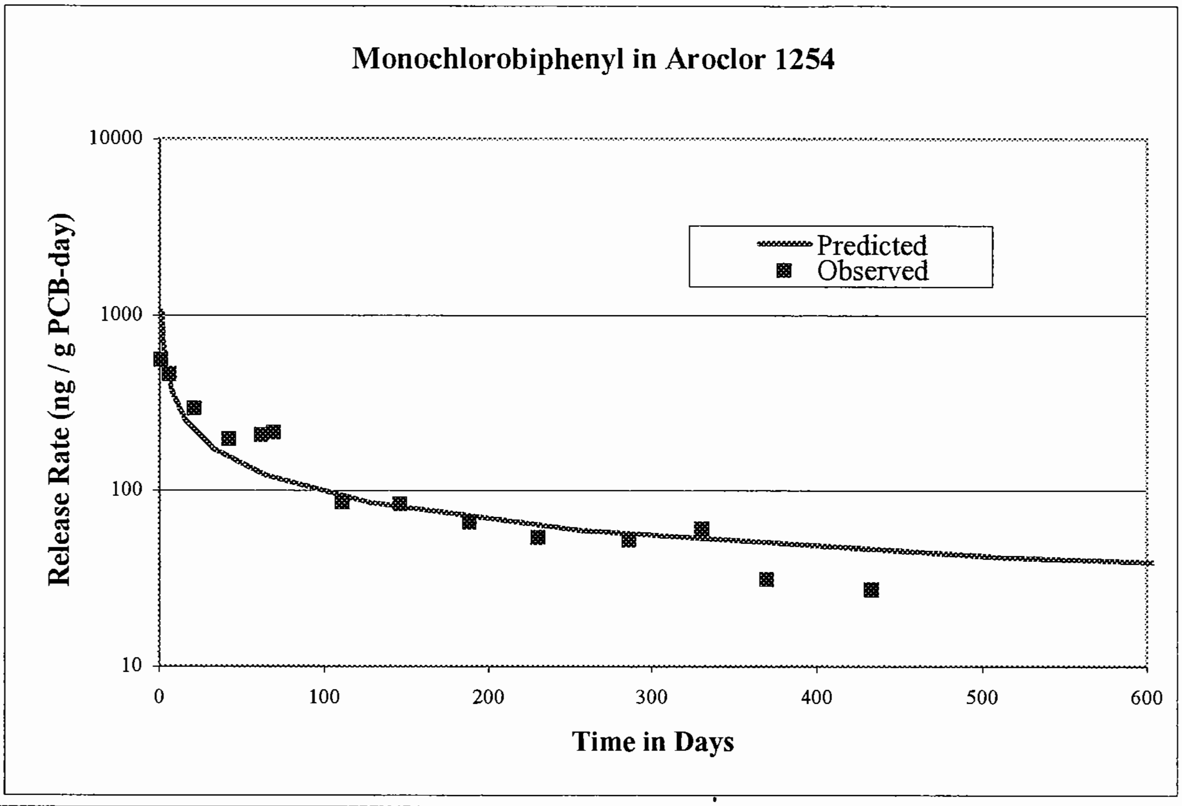
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.04E+01	1.04E+01	7.26E+01	1.97E-06
Residual	12	1.73E+00	1.44E-01		
Total	13	1.22E+01			

	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	6.96E+00	2.83E-01	2.46E+01	1.21E-11	6.34E+00	7.57E+00
ln(day)	-5.17E-01	6.07E-02	-8.52E+00	1.97E-06	-6.49E-01	-3.85E-01

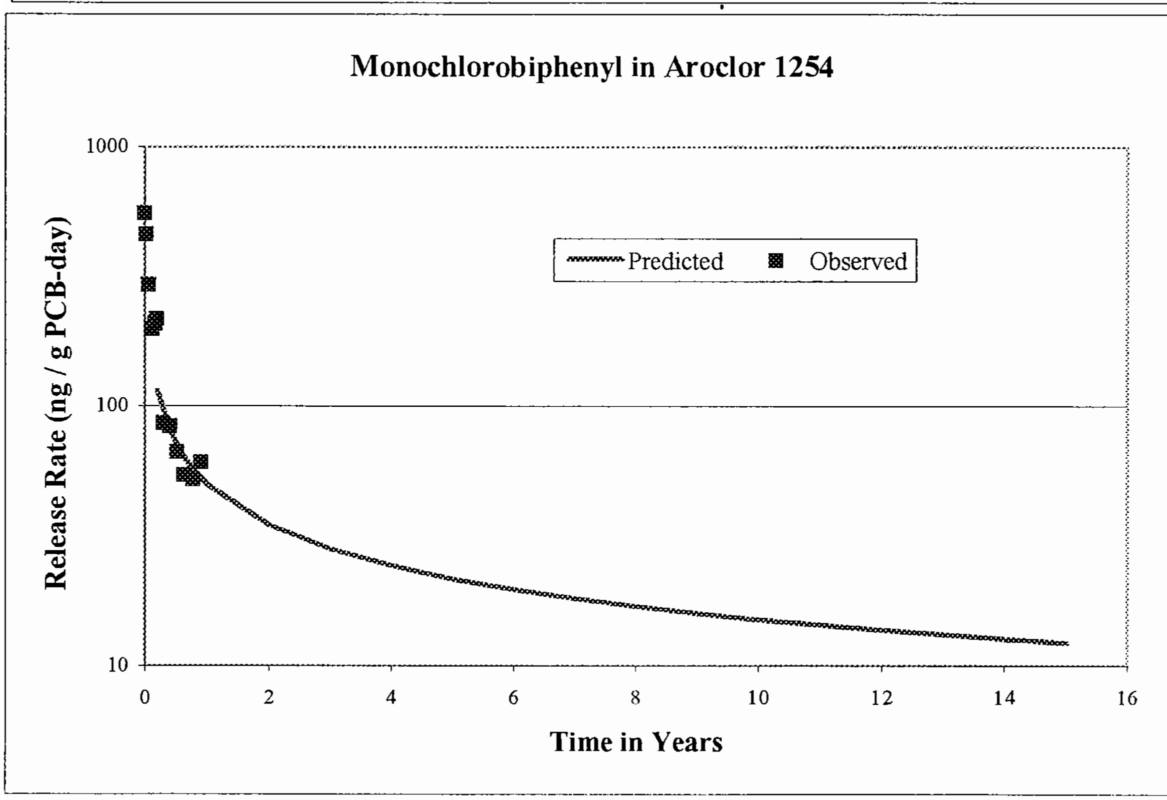
RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	6.94E+00	-6.28E-01
2	6.03E+00	1.04E-01
3	5.38E+00	3.03E-01
4	5.02E+00	2.61E-01
5	4.82E+00	5.11E-01
6	4.77E+00	6.03E-01
7	4.52E+00	-7.24E-02
8	4.38E+00	4.13E-02
9	4.25E+00	-5.79E-02
10	4.14E+00	-1.56E-01

Observatiordicted ln(ng/g-PCI		*Residuals*
11	4.03E+00	-8.23E-02
12	3.96E+00	1.45E-01
13	3.90E+00	-4.58E-01
14	3.82E+00	-5.15E-01



Monochlorobiphenyl in Aroclor 1254
Predicted
Observed
Release Rate (ng / g PCB-day)
10000
1000
100
10
0
100
200
300
400
500
600
Time in Days



Monochlorobiphenyl in Aroclor 1254
Predicted
Observed
Release Rate (ng / g PCB-day)
1000
100
10
0
2
4
6
8
10
12
14
16
Time in Years

Dichlorobiphenyl in Aroclor 1254

ng/ g-PCB - d	Cl2
2.08E-03	0
1.03E+00	1576
6.06E+00	1213
2.13E+01	877
4.23E+01	643
6.21E+01	646
6.93E+01	797
1.11E+02	344
1.46E+02	340
1.88E+02	262
2.30E+02	249
2.86E+02	205
3.31E+02	278
3.70E+02	190
4.33E+02	139

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
2.54E-02	1.03E+00	1576	7.36E+00
1.80E+00	6.06E+00	1213	7.10E+00
3.06E+00	2.13E+01	877	6.78E+00
3.74E+00	4.23E+01	643	6.47E+00
4.13E+00	6.21E+01	646	6.47E+00
4.24E+00	6.93E+01	797	6.68E+00
4.71E+00	1.11E+02	344	5.84E+00
4.98E+00	1.46E+02	340	5.83E+00
5.24E+00	1.88E+02	262	5.57E+00
5.44E+00	2.30E+02	249	5.52E+00
5.66E+00	2.86E+02	205	5.32E+00
5.80E+00	3.31E+02	278	5.63E+00
5.91E+00	3.70E+02	190	5.24E+00
6.07E+00	4.33E+02	139	4.94E+00

Maximum Release Rate at 1 day
1576 ng/gPCB-d

Release rate at 2 years
172 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.9281
R Square	0.8614
Standard Error	0.2904
Observations	14

ANOVA

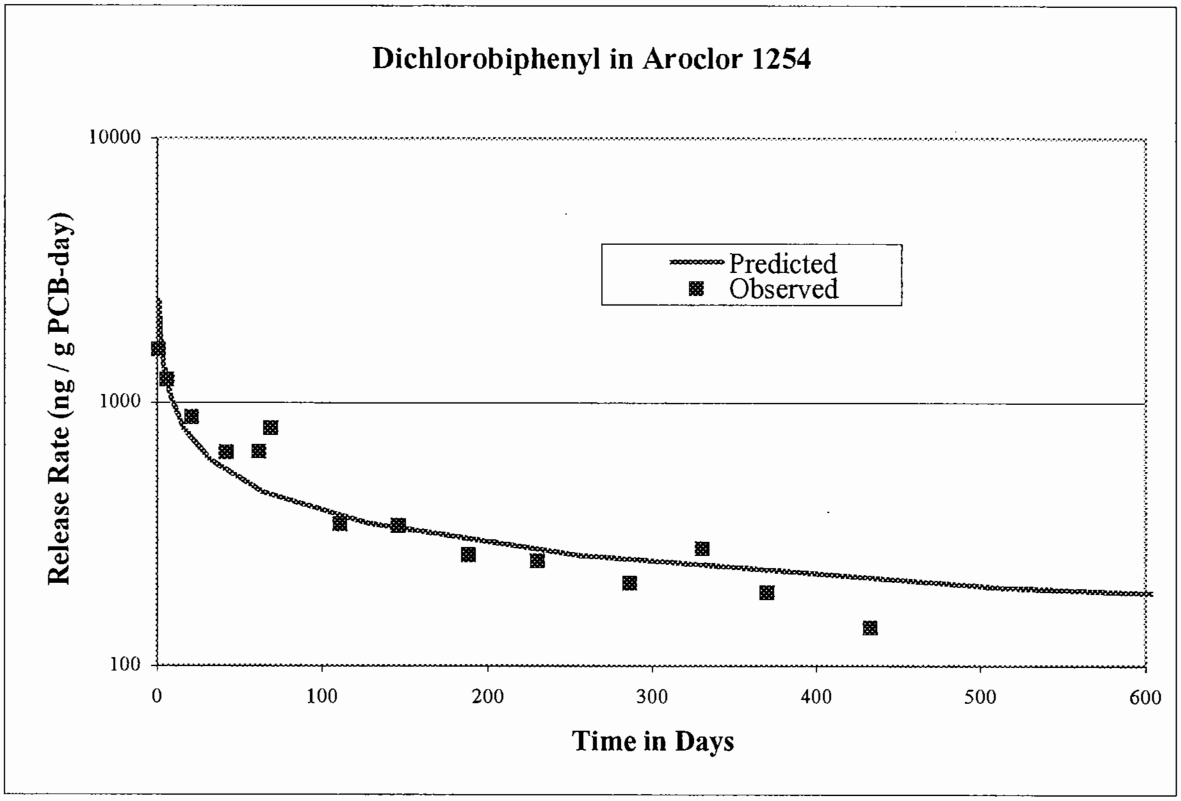
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	6.29E+00	6.29E+00	7.46E+01	1.70E-06
Residual	12	1.01E+00	8.44E-02		
Total	13	7.31E+00			

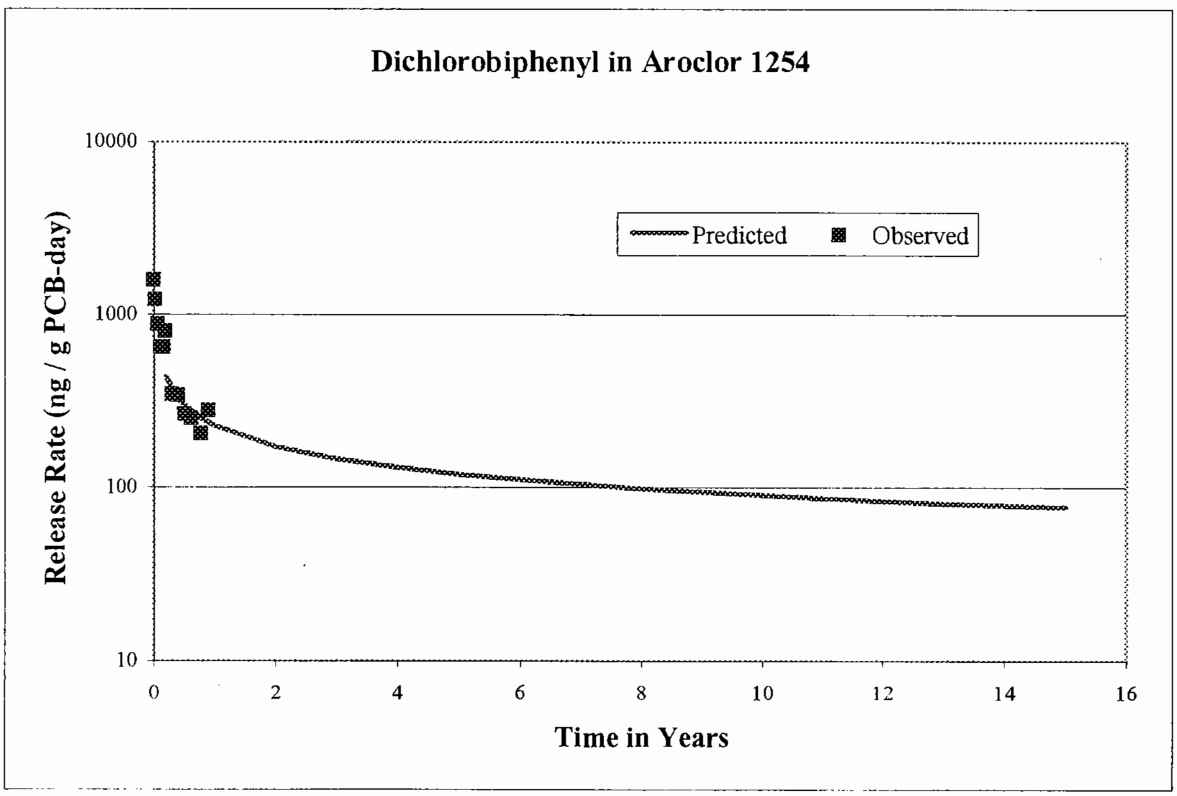
	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	7.80E+00	2.16E-01	3.60E+01	1.33E-13	7.33E+00	8.27E+00
ln(day)	-4.02E-01	4.65E-02	-8.64E+00	1.70E-06	-5.03E-01	-3.00E-01

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	7.79E+00	-4.25E-01
2	7.07E+00	2.68E-02
3	6.57E+00	2.07E-01
4	6.29E+00	1.72E-01
5	6.14E+00	3.31E-01
6	6.10E+00	5.85E-01
7	5.91E+00	-6.46E-02
8	5.80E+00	3.38E-02
9	5.69E+00	-1.25E-01
10	5.61E+00	-9.50E-02

Observation	*dicted ln(ng/g-PCI*	*Residuals*
11	5.53E+00	-2.05E-01
12	5.47E+00	1.58E-01
13	5.42E+00	-1.78E-01
14	5.36E+00	-4.22E-01


Dichlorobiphenyl in Aroclor 1254
Predicted
Observed
10000
1000
100
0
100
200
300
400
500
600
Release Rate (ng / g PCB-day)
Time in Days


Dichlorobiphenyl in Aroclor 1254
Predicted
Observed
10000
1000
100
10
0
2
4
6
8
10
12
14
16
Release Rate (ng / g PCB-day)
Time in Years

Trichlorobiphenyl in Aroclor 1254

ng/ g-PCB - d	Cl3
2.08E-03	0
1.03E+00	511
6.06E+00	849
2.13E+01	702
4.23E+01	562
6.21E+01	623
6.93E+01	1103
1.11E+02	344
1.46E+02	353
1.88E+02	273
2.30E+02	301
2.86E+02	173
3.31E+02	248
3.70E+02	190
4.33E+02	132

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
4.24E+00	6.93E+01	1103	7.01E+00
4.71E+00	1.11E+02	344	5.84E+00
4.98E+00	1.46E+02	353	5.87E+00
5.24E+00	1.88E+02	273	5.61E+00
5.44E+00	2.30E+02	301	5.71E+00
5.66E+00	2.86E+02	173	5.15E+00
5.80E+00	3.31E+02	248	5.51E+00
5.91E+00	3.70E+02	190	5.24E+00
6.07E+00	4.33E+02	132	4.89E+00

Maximum Release Rate at 69 days
1103 ng/gPCB-d

Release rate at 2 years
89.7 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.9169
R Square	0.8407
Standard Error	0.2587
Observations	9

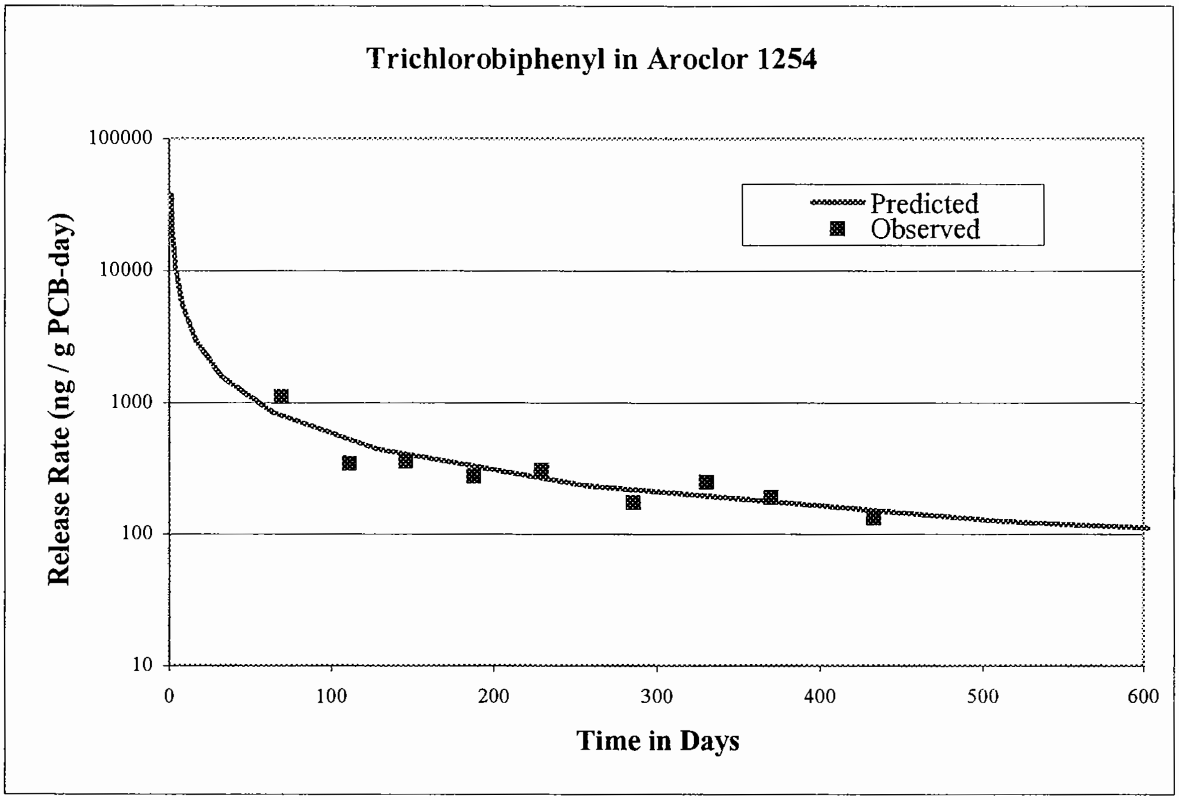
ANOVA

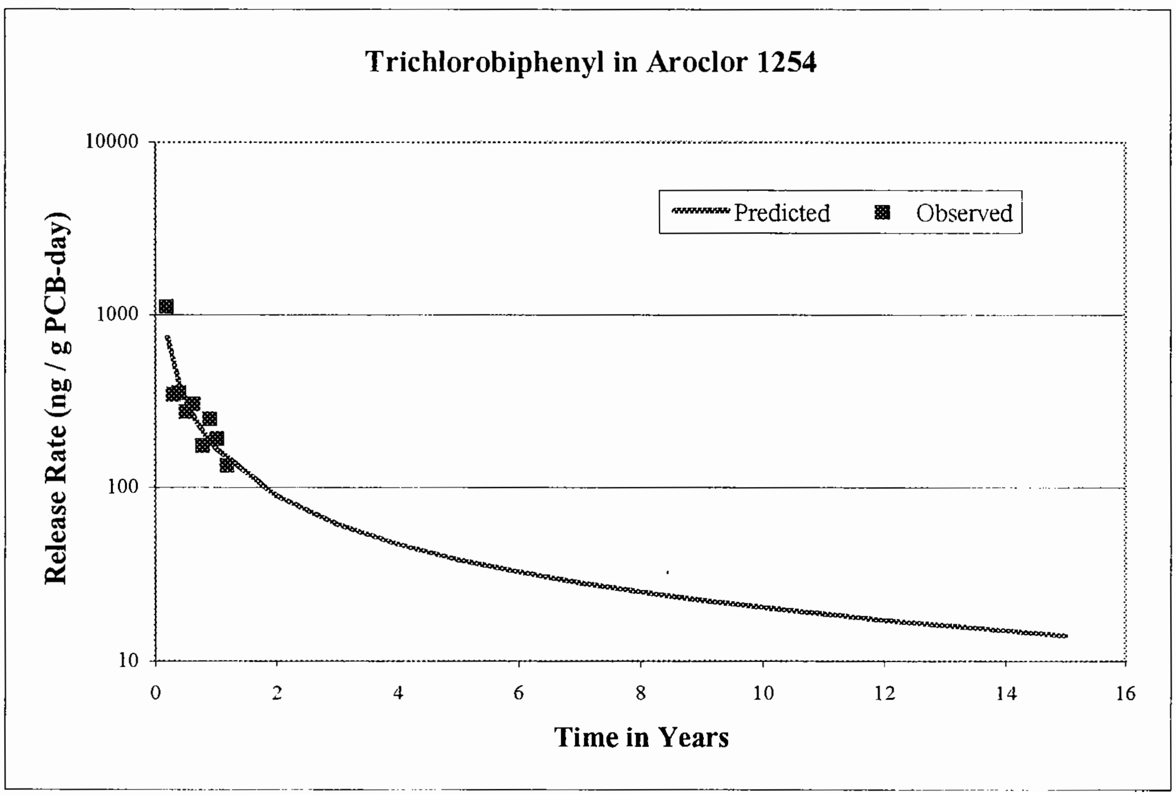
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	2.47E+00	2.47E+00	3.69E+01	5.02E-04
Residual	7	4.68E-01	6.69E-02		
Total	8	2.94E+00			

	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	1.05E+01	8.11E-01	1.30E+01	3.69E-06	8.63E+00	1.25E+01
ln(day)	-9.18E-01	1.51E-01	-6.08E+00	5.02E-04	-1.27E+00	-5.61E-01

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	6.66E+00	3.48E-01
2	6.22E+00	-3.83E-01
3	5.97E+00	-1.07E-01
4	5.74E+00	-1.32E-01
5	5.56E+00	1.52E-01
6	5.36E+00	-2.02E-01
7	5.22E+00	2.89E-01
8	5.12E+00	1.25E-01
9	4.98E+00	-8.90E-02


Trichlorobiphenyl in Aroclor 1254
Release Rate (ng / g PCB-day)
Time in Days
Predicted
Observed
100000
10000
1000
100
10
0
100
200
300
400
500
600


Trichlorobiphenyl in Aroclor 1254
Release Rate (ng / g PCB-day)
Time in Years
Predicted
Observed
10000
1000
100
10
0
2
4
6
8
10
12
14
16

Tetrachlorobiphenyl in Aroclor 1254

ng/ g-PCB - d	Cl4
2.08E-03	0
1.03E+00	1278
6.06E+00	5373
2.13E+01	6726
4.23E+01	7630
6.21E+01	8461
6.93E+01	22679
1.11E+02	5737
1.46E+02	6049
1.88E+02	3357
2.30E+02	6128
2.86E+02	2517
3.31E+02	3173
3.70E+02	2565
4.33E+02	1882

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
4.24E+00	6.93E+01	22679	1.00E+01
4.71E+00	1.11E+02	5737	8.65E+00
4.98E+00	1.46E+02	6049	8.71E+00
5.24E+00	1.88E+02	3357	8.12E+00
5.44E+00	2.30E+02	6128	8.72E+00
5.66E+00	2.86E+02	2517	7.83E+00
5.80E+00	3.31E+02	3173	8.06E+00
5.91E+00	3.70E+02	2565	7.85E+00
6.07E+00	4.33E+02	1882	7.54E+00

Maximum Release Rate at 69 days
22679 ng/gPCB-d

Release rate at 2 years
1082 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.9065
R Square	0.8218
Standard Error	0.3375
Observations	9

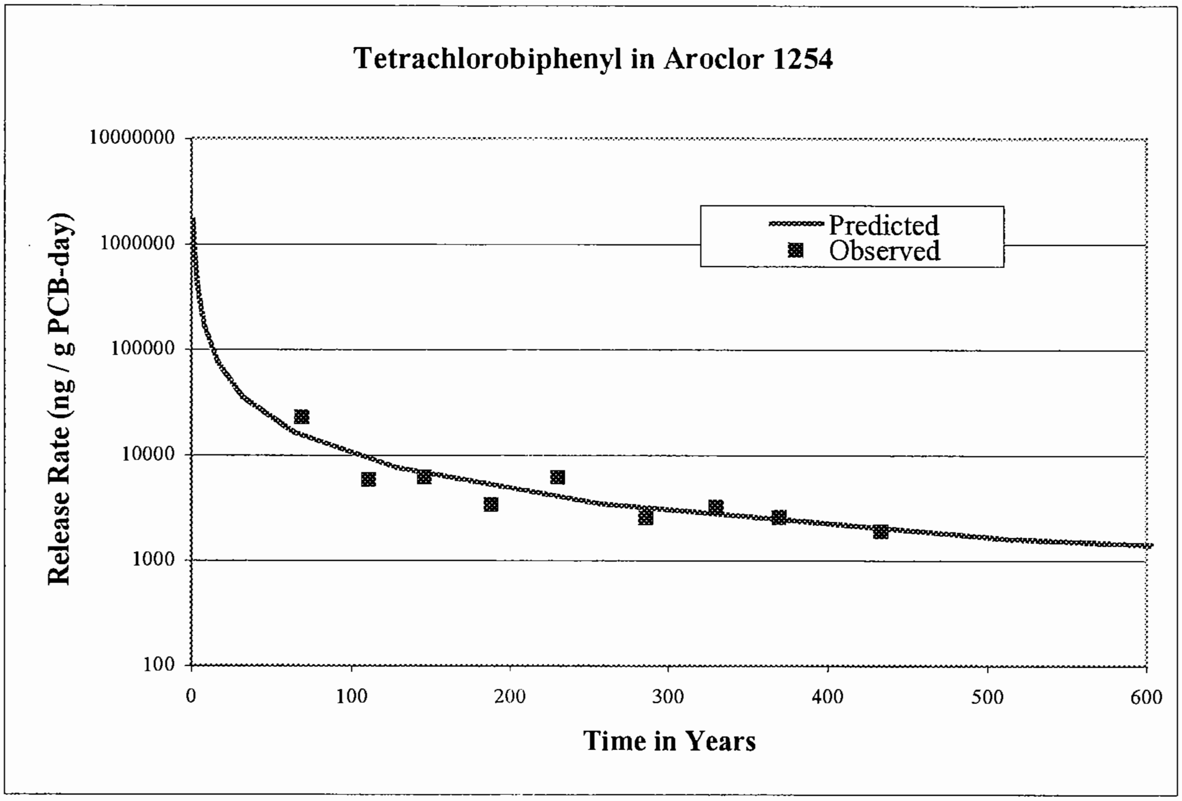
ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	3.68E+00	3.68E+00	3.23E+01	7.49E-04
Residual	7	7.97E-01	1.14E-01		
Total	8	4.47E+00			

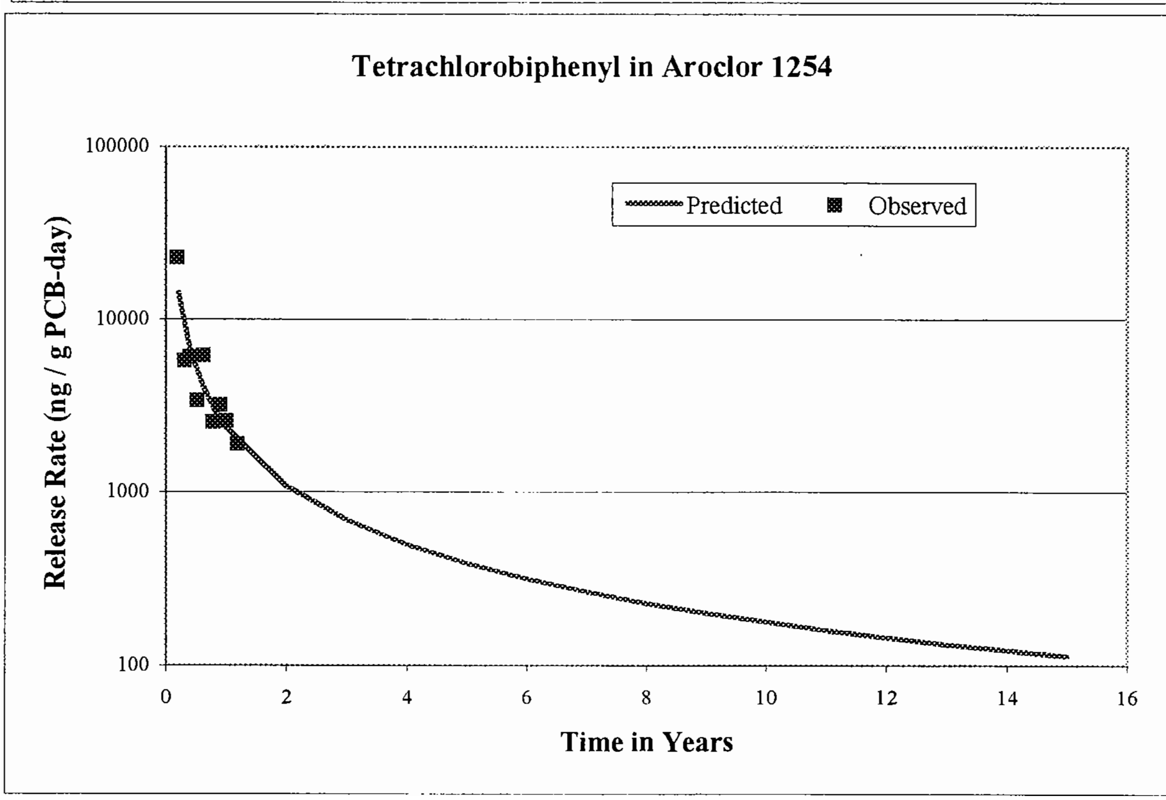
	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	1.44E+01	1.06E+00	1.36E+01	2.76E-06	1.19E+01	1.69E+01
ln(day)	-1.12E+00	1.97E-01	-5.68E+00	7.49E-04	-1.59E+00	-6.54E-01

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	9.62E+00	4.06E-01
2	9.09E+00	-4.39E-01
3	8.79E+00	-8.00E-02
4	8.50E+00	-3.86E-01
5	8.28E+00	4.41E-01
6	8.04E+00	-2.04E-01
7	7.87E+00	1.89E-01
8	7.75E+00	1.03E-01
9	7.57E+00	-3.02E-02



Tetrachlorobiphenyl in Aroclor 1254
Release Rate (ng / g PCB-day)
10000000
1000000
100000
10000
1000
100
0
100
200
300
400
500
600
Time in Years
Predicted
Observed



Tetrachlorobiphenyl in Aroclor 1254
Release Rate (ng / g PCB-day)
100000
10000
1000
100
0
2
4
6
8
10
12
14
16
Time in Years
Predicted
Observed

Pentachlorobiphenyl in Aroclor 1254

ng/ g-PCB - d	Cl5
2.08E-03	0
1.03E+00	0
6.06E+00	1127
2.13E+01	2778
4.23E+01	5020
6.21E+01	6902
6.93E+01	26356
1.11E+02	5320
1.46E+02	5167
1.88E+02	3043
2.30E+02	8620
2.86E+02	2124
3.31E+02	2380
3.70E+02	1561
4.33E+02	1185

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
4.24E+00	6.93E+01	26356	1.02E+01
4.71E+00	1.11E+02	5320	8.58E+00
4.98E+00	1.46E+02	5167	8.55E+00
5.24E+00	1.88E+02	3043	8.02E+00
5.44E+00	2.30E+02	8620	9.06E+00
5.66E+00	2.86E+02	2124	7.66E+00
5.80E+00	3.31E+02	2380	7.77E+00
5.91E+00	3.70E+02	1561	7.35E+00
6.07E+00	4.33E+02	1185	7.08E+00

Maximum Release Rate at 69 days
26356 ng/gPCB-d

Release rate at 2 years
660 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.8838
R Square	0.7811
Standard Error	0.4806
Observations	9

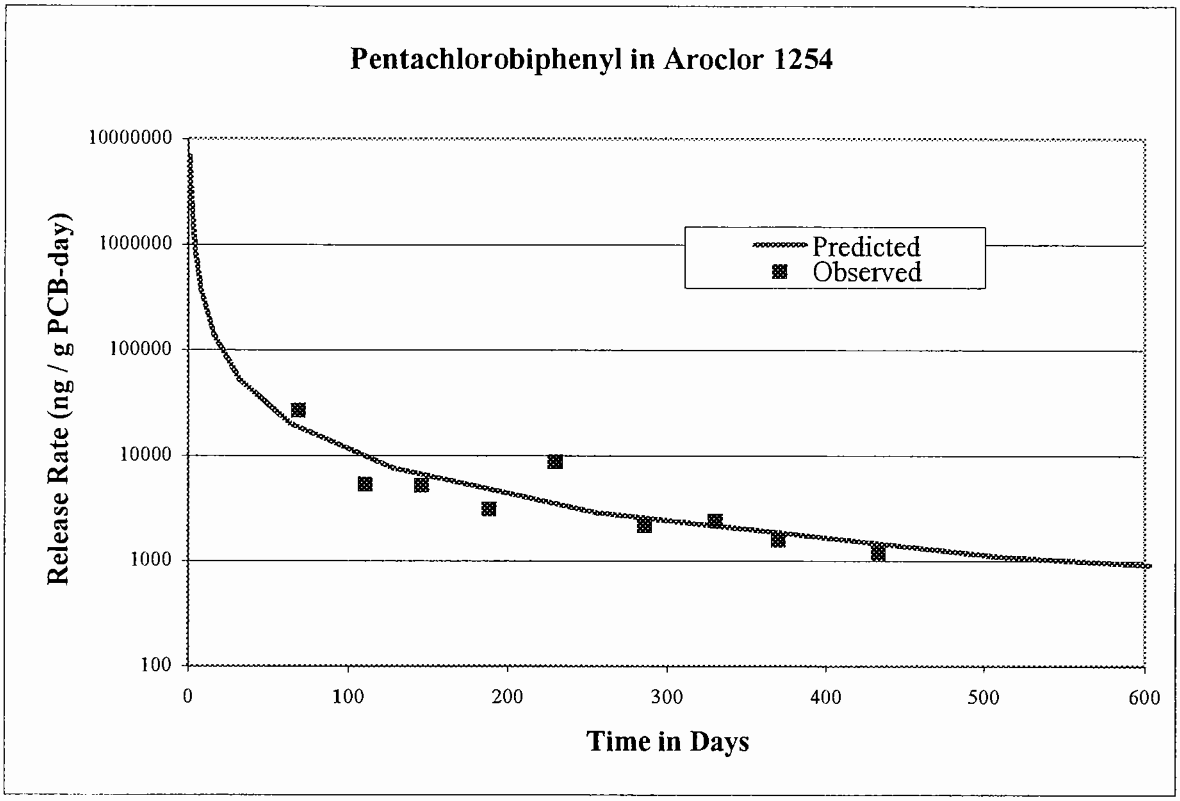
ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	5.77E+00	5.77E+00	2.50E+01	1.57E-03
Residual	7	1.62E+00	2.31E-01		
Total	8	7.38E+00			

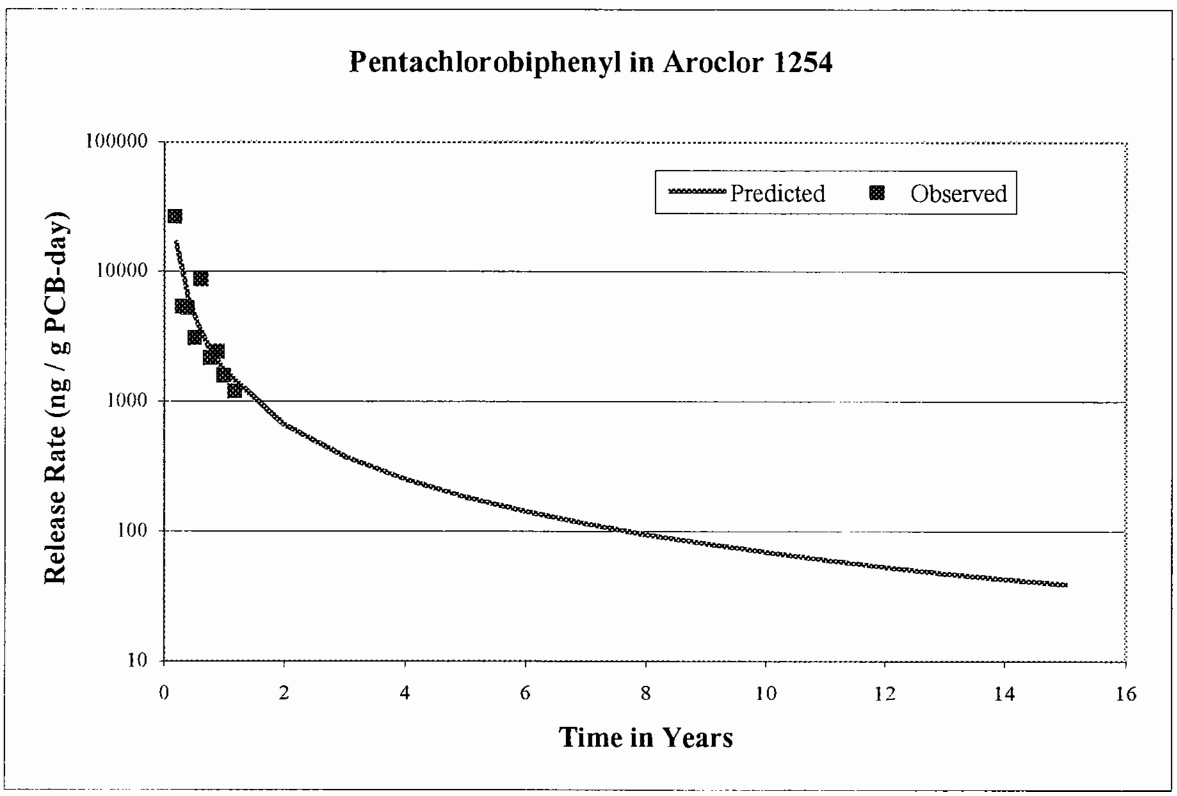
	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	1.57E+01	1.51E+00	1.04E+01	1.60E-05	1.22E+01	1.93E+01
ln(day)	-1.40E+00	2.81E-01	-5.00E+00	1.57E-03	-2.07E+00	-7.39E-01

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	9.79E+00	3.85E-01
2	9.13E+00	-5.53E-01
3	8.75E+00	-1.98E-01
4	8.39E+00	-3.73E-01
5	8.11E+00	9.50E-01
6	7.81E+00	-1.45E-01
7	7.60E+00	1.71E-01
8	7.44E+00	-9.17E-02
9	7.22E+00	-1.46E-01



Pentachlorobiphenyl in Aroclor 1254
Release Rate (ng / g PCB-day)
10000000
1000000
100000
10000
1000
100
Predicted
Observed
0
100
200
300
400
500
600
Time in Days



Pentachlorobiphenyl in Aroclor 1254
Release Rate (ng / g PCB-day)
100000
10000
1000
100
10
Predicted
Observed
0
2
4
6
8
10
12
14
16
Time in Years

Hexachlorobiphenyl in Aroclor 1254

ng/ g-PCB - d	Cl6
2.08E-03	0
1.03E+00	0
6.06E+00	0
2.13E+01	88
4.23E+01	321
6.21E+01	534
6.93E+01	2636
1.11E+02	678
1.46E+02	555
1.88E+02	399
2.30E+02	1246
2.86E+02	370
3.31E+02	347
3.70E+02	156
4.33E+02	139

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
4.24E+00	6.93E+01	2636	7.88E+00
4.71E+00	1.11E+02	678	6.52E+00
4.98E+00	1.46E+02	555	6.32E+00
5.24E+00	1.88E+02	399	5.99E+00
5.44E+00	2.30E+02	1246	7.13E+00
5.66E+00	2.86E+02	370	5.91E+00
5.80E+00	3.31E+02	347	5.85E+00
5.91E+00	3.70E+02	156	5.05E+00
6.07E+00	4.33E+02	139	4.94E+00

Maximum Release Rate at 69 days
2636 ng/gPCB-d

Release rate at 2 years
94.2 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.8445
R Square	0.7131
Standard Error	0.5337
Observations	9

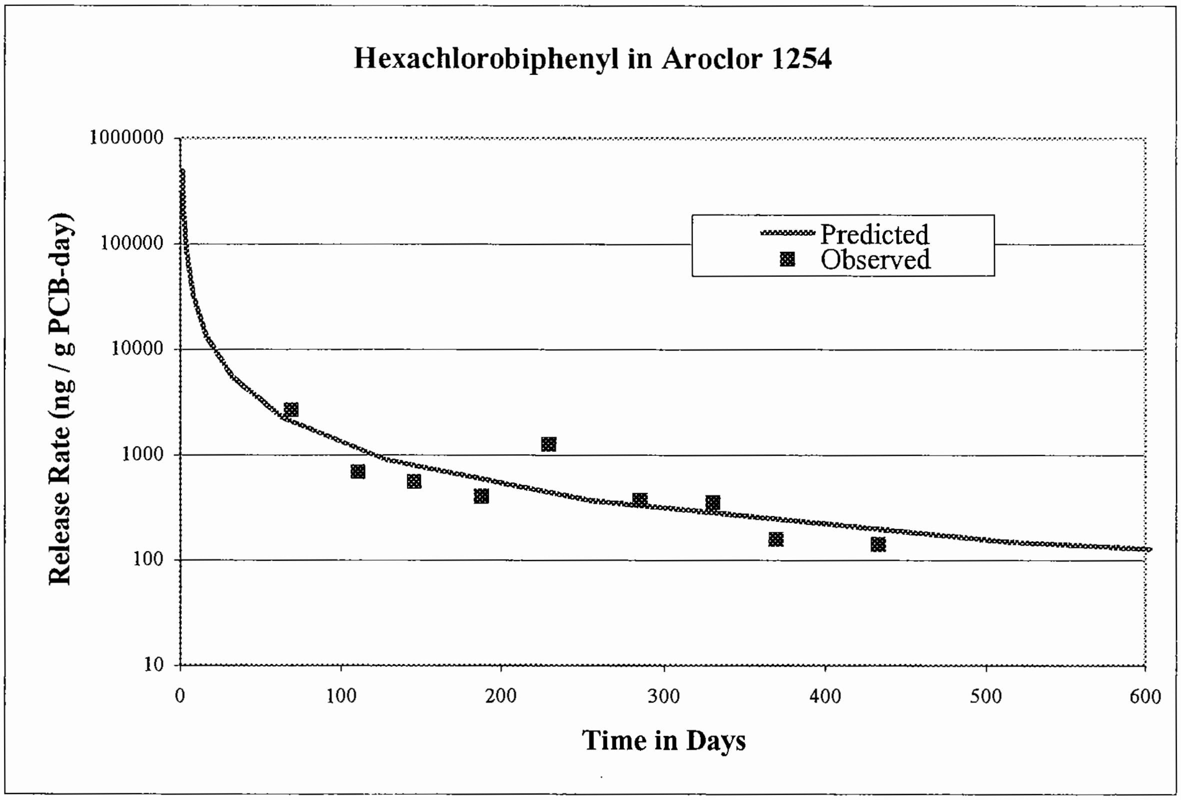
ANOVA

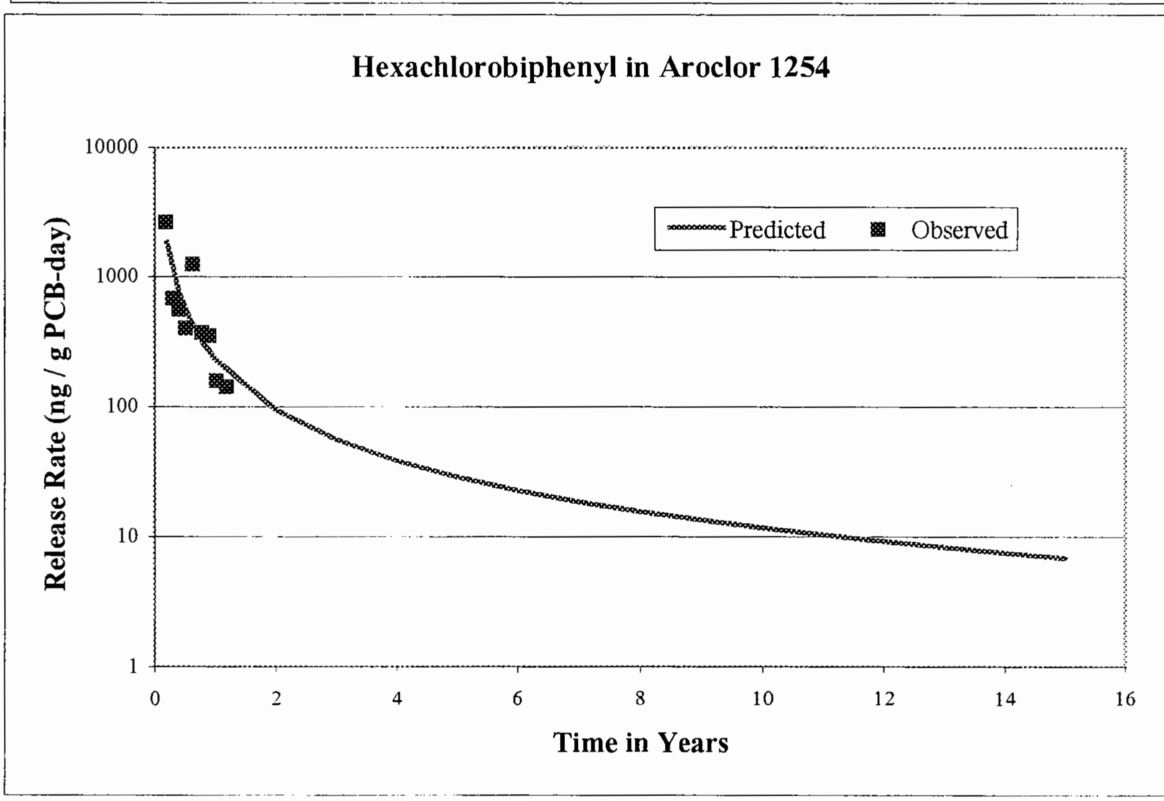
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	4.96E+00	4.96E+00	1.74E+01	4.18E-03
Residual	7	1.99E+00	2.85E-01		
Total	8	6.95E+00			

	Coefficients	*andard Errı*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	1.31E+01	1.67E+00	7.84E+00	1.04E-04	9.16E+00	1.71E+01
ln(day)	-1.30E+00	3.12E-01	-4.17E+00	4.18E-03	-2.04E+00	-5.63E-01

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	7.61E+00	2.71E-01
2	6.99E+00	-4.73E-01
3	6.64E+00	-3.19E-01
4	6.31E+00	-3.20E-01
5	6.05E+00	1.08E+00
6	5.76E+00	1.50E-01
7	5.58E+00	2.74E-01
8	5.43E+00	-3.78E-01
9	5.22E+00	-2.86E-01


Hexachlorobiphenyl in Aroclor 1254
Release Rate (ng / g PCB-day)
1000000
100000
10000
1000
100
10
0
100
200
300
400
500
600
Time in Days
Predicted
Observed


Hexachlorobiphenyl in Aroclor 1254
Release Rate (ng / g PCB-day)
10000
1000
100
10
1
0
2
4
6
8
10
12
14
16
Time in Years
Predicted
Observed

BLACK RUBBER MATERIAL

Black Rubber Material

Leaching Time (days)	Homologue Leach Rates (ng PCB/g shipboard solid-day)									
	Cl1	Cl2	Cl3	Cl4	Cl5	Cl6	Cl7	Cl8	Cl9	Cl10
0.006	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	2.7E+02	0.0E+00	0.0E+00	0.0E+00
1.169	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	1.3E+00	0.0E+00	0.0E+00	0.0E+00
7.074	2.9E-01	8.0E-01	3.4E-01	1.2E+00	9.6E-01	0.0E+00	5.0E-01	0.0E+00	0.0E+00	0.0E+00
14.081	0.0E+00	2.0E+00	3.8E-01	1.5E+00	7.4E-01	0.0E+00	3.5E-01	0.0E+00	0.0E+00	0.0E+00
28.153	1.9E-01	2.5E-01	2.3E-01	1.1E+00	9.2E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
49.204	1.5E-01	2.4E-02	1.2E-01	1.0E+00	6.1E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
69.272	0.0E+00	2.3E-02	1.8E-01	1.4E+00	1.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
104.181	1.3E-01	1.6E-01	1.3E-01	7.8E-01	7.3E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
146.122	1.1E-01	1.5E-01	1.6E-01	6.6E-01	6.6E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
188.072	9.1E-02	9.1E-02	9.9E-02	4.7E-01	4.0E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
230.109	8.3E-02	9.8E-03	3.5E-01	4.4E-01	4.0E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
286.142	1.0E-01	1.2E-02	2.6E-01	2.2E-01	8.5E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
328.083	9.1E-02	5.6E-02	5.3E-02	2.9E-01	2.1E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
370.110	9.1E-02	8.4E-02	7.3E-02	3.3E-01	1.7E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
398.072	8.1E-02	1.8E-01	1.4E-01	4.3E-01	3.5E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
475.124	7.0E-02	5.4E-02	9.1E-02	2.6E-01	1.8E-01	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
Max	2.9E-01	2.0E+00	3.8E-01	1.5E+00	1.0E+00	0.0E+00	2.7E+02	0.0E+00	0.0E+00	0.0E+00
Min	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00

0.0016 g PCB / g rubber material (leachate study concentration)

Leaching Time (days)	Homologue Leach Rates (ng PCB/g PCB-day)									
ng/ g-PCB - d	Cl1	Cl2	Cl3	Cl4	Cl5	Cl6	Cl7	Cl8	Cl9	Cl10
0.006	0	0	0	0	0	0	167503	0	0	0
1.169	0	0	0	0	0	0	833	0	0	0
7.074	184	502	211	736	602	0	311	0	0	0
14.081	0	1267	239	922	461	0	222	0	0	0
28.153	119	158	143	688	574	0	0	0	0	0
49.204	93	15	78	654	379	0	0	0	0	0
69.272	0	14	114	895	638	0	0	0	0	0
104.181	80	97	80	486	458	0	0	0	0	0
146.122	67	91	101	414	414	0	0	0	0	0
188.072	57	57	62	295	248	0	0	0	0	0
230.109	52	6	216	273	249	0	0	0	0	0
286.142	63	7	162	137	53	0	0	0	0	0
328.083	57	35	33	181	129	0	0	0	0	0
370.110	57	52	46	204	109	0	0	0	0	0
398.072	51	114	86	271	221	0	0	0	0	0
475.124	44	34	57	163	111	0	0	0	0	0
Max	184	1267	239	922	638	0	167503	0	0	0
Min	0	0	0	0	0	0	0	0	0	0
Median	57.1	43.5	82.9	284	248	0	0	0	0	0
Simple Average	57.8	153	102	395	290	0	10554	0	0	0
Number of detects	12	14	14	14	14	0	4	0	0	0
Number of nondetects	4	2	2	2	2	16	12	16	16	16
intercept	5.81E+00	7.09E+00	5.99E+00	8.50E+00	1.07E+01	---	7.40E+00	---	---	---
slope	-3.17E-01	-6.55E-01	-2.97E-01	-5.36E-01	-9.95E-01	---	-8.78E-01	---	---	---
alpha	2.88E-08	7.83E-02	4.98E-02	2.22E-05	4.47E-03	---	7.51E-03	---	---	---

Monochlorobiphenyl in Bulkhead Insulation

ng/ g-PCB - d	Cl1
6.25E-03	0
1.17E+00	0
7.07E+00	184
1.41E+01	0
2.82E+01	119
4.92E+01	93.0
6.93E+01	0
1.04E+02	80.1
1.46E+02	67.4
1.88E+02	57.1
2.30E+02	51.7
2.86E+02	63.5
3.28E+02	57.1
3.70E+02	57.0
3.98E+02	50.7
4.75E+02	44.1

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
1.96E+00	7.07E+00	184	5.21E+00
3.34E+00	2.82E+01	119	4.78E+00
3.90E+00	4.92E+01	93	4.53E+00
4.65E+00	1.04E+02	80	4.38E+00
4.98E+00	1.46E+02	67	4.21E+00
5.24E+00	1.88E+02	57	4.05E+00
5.44E+00	2.30E+02	52	3.95E+00
5.66E+00	2.86E+02	63	4.15E+00
5.79E+00	3.28E+02	57	4.05E+00
5.91E+00	3.70E+02	57	4.04E+00
5.99E+00	3.98E+02	51	3.93E+00
6.16E+00	4.75E+02	44	3.79E+00

Maximum Release Rate at 7 days
184 ng/gPCB-d

Release rate at 2 years
41.4 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.9793
R Square	0.9591
Standard Error	0.0873
Observations	12

ANOVA

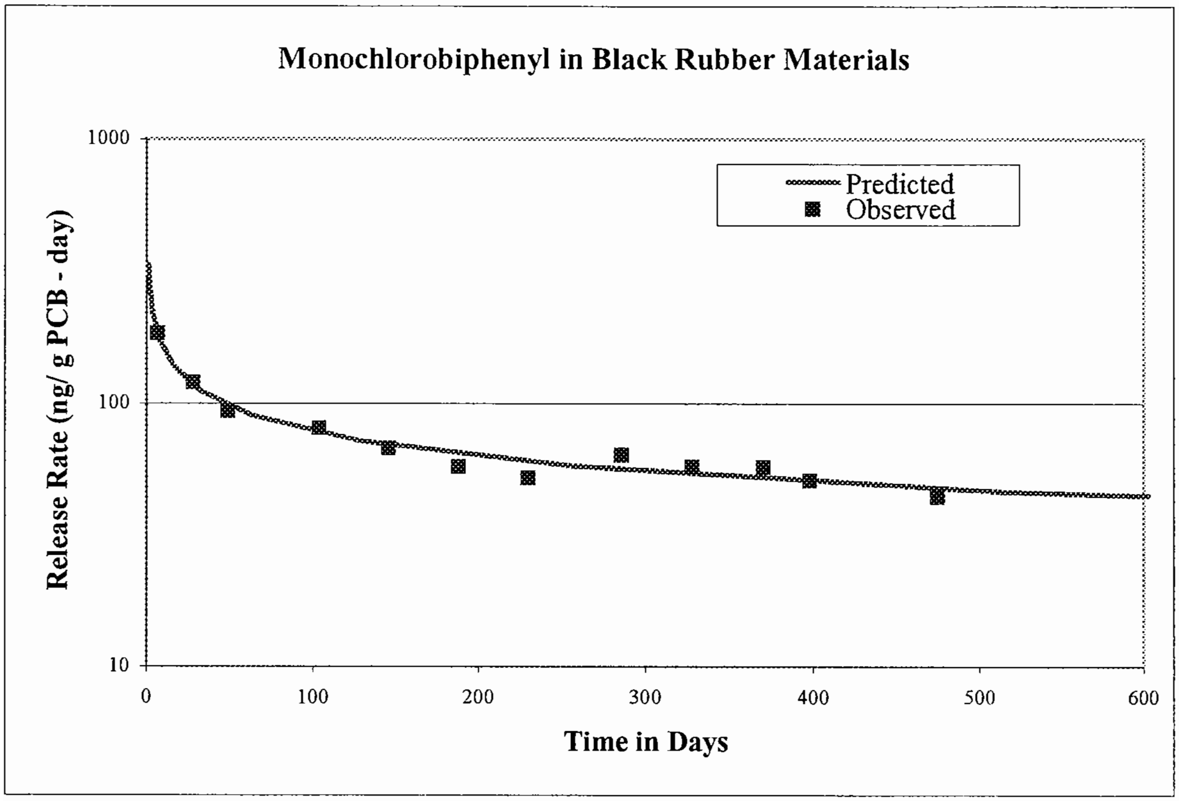
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.78E+00	1.78E+00	2.34E+02	2.88E-08
Residual	10	7.61E-02	7.61E-03		
Total	11	1.86E+00			

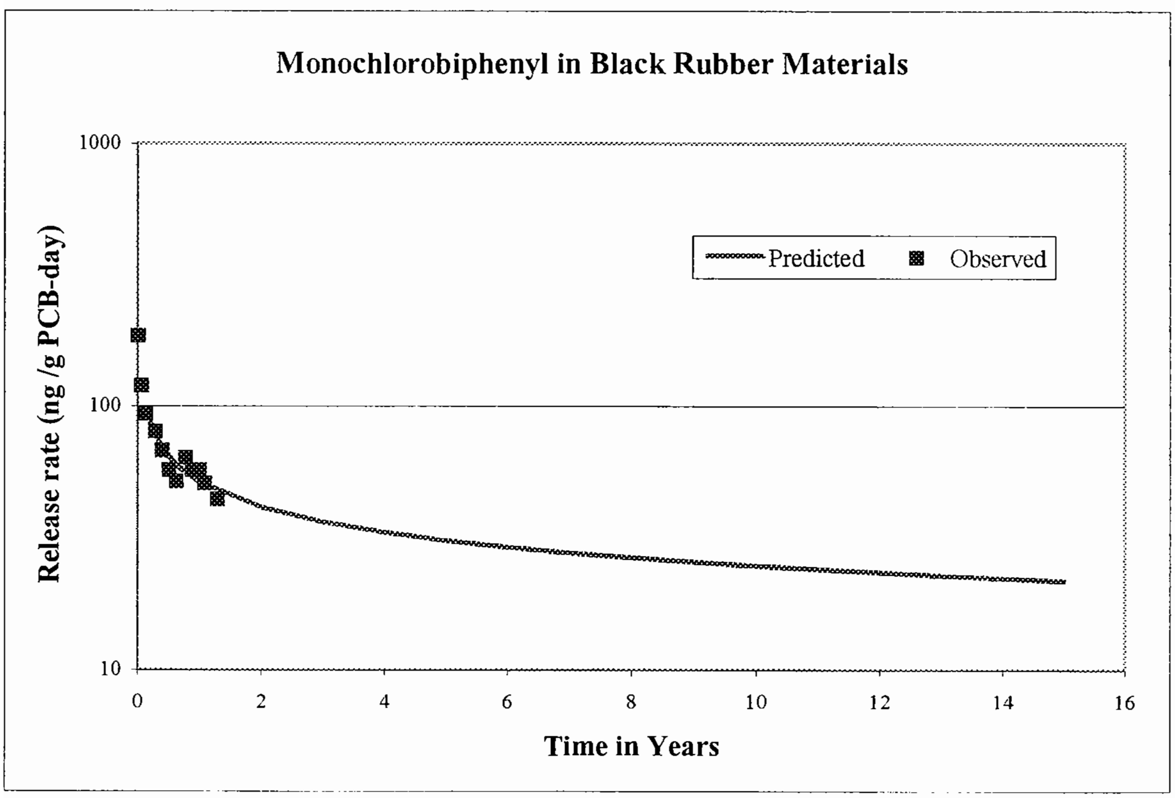
	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	5.81E+00	1.05E-01	5.54E+01	8.85E-14	5.58E+00	6.05E+00
ln(day)	-3.17E-01	2.07E-02	-1.53E+01	2.88E-08	-3.63E-01	-2.71E-01

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	5.19E+00	2.14E-02
2	4.76E+00	2.37E-02
3	4.58E+00	-4.67E-02
4	4.34E+00	4.20E-02
5	4.23E+00	-2.36E-02
6	4.15E+00	-1.09E-01
7	4.09E+00	-1.45E-01
8	4.02E+00	1.30E-01
9	3.98E+00	6.79E-02
10	3.94E+00	1.04E-01
11	3.92E+00	9.75E-03

12	3.86E+00	-7.47E-02





Dichlorobiphenyl in Bulkhead Insulation

ng/ g-PCB - d	Cl2
6.25E-03	0
1.17E+00	0
7.07E+00	502
1.41E+01	1267
2.82E+01	158
4.92E+01	15.2
6.93E+01	14
1.04E+02	97.2
1.46E+02	91.4
1.88E+02	57.1
2.30E+02	6.1
2.86E+02	7.4
3.28E+02	34.8
3.70E+02	52.3
3.98E+02	114
4.75E+02	33.7

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
2.64E+00	1.41E+01	1267	7.14E+00
3.34E+00	2.82E+01	158	5.06E+00
3.90E+00	4.92E+01	15	2.72E+00
4.24E+00	6.93E+01	14	2.66E+00
4.65E+00	1.04E+02	97	4.58E+00
4.98E+00	1.46E+02	91	4.52E+00
5.24E+00	1.88E+02	57	4.05E+00
5.44E+00	2.30E+02	6	1.81E+00
5.66E+00	2.86E+02	7	2.00E+00
5.79E+00	3.28E+02	35	3.55E+00
5.91E+00	3.70E+02	52	3.96E+00
5.99E+00	3.98E+02	114	4.74E+00
6.16E+00	4.75E+02	34	3.52E+00

Maximum Release Rate at 14 days
1267 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.5051
R Square	0.2552
Standard Error	1.2907
Observations	13

ANOVA

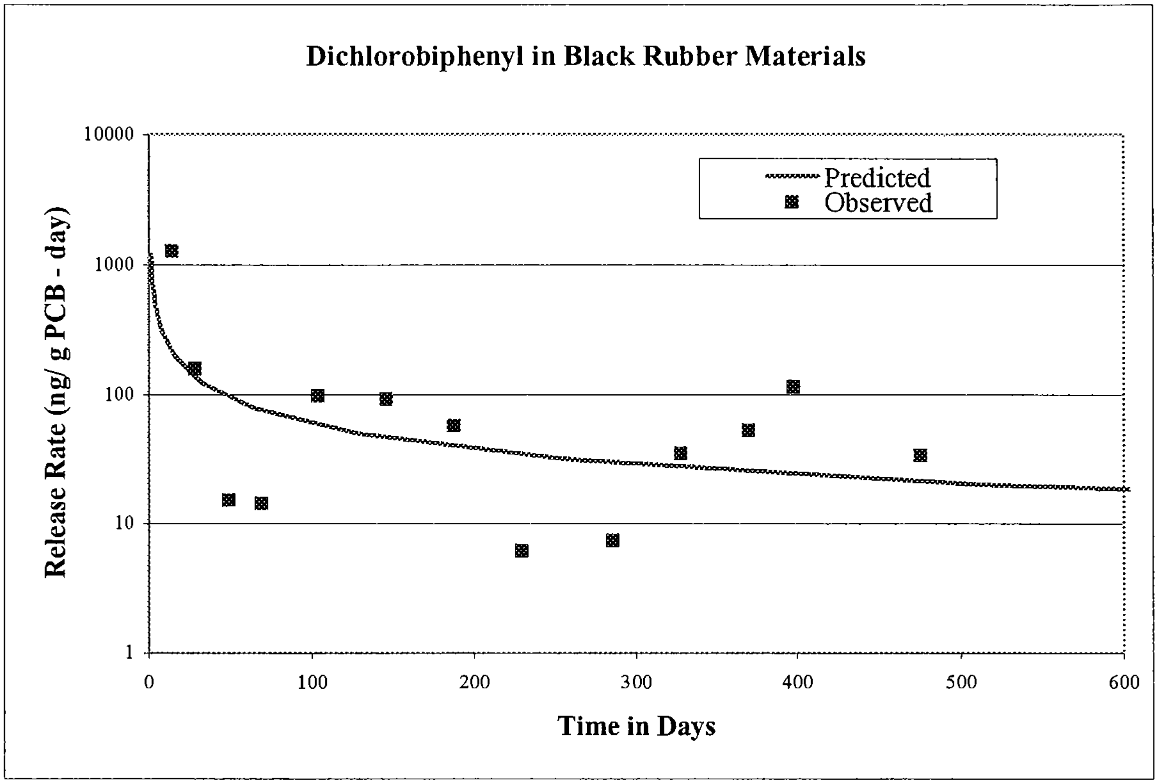
	df	*SS*	*MS*	*F*	*Significance F*	
Regression	1	6.28E+00	6.28E+00	3.77E+00	7.83E-02	***Not Significant***
Residual	11	1.83E+01	1.67E+00			
Total	12	2.46E+01				

	Coefficients	*andard Erro*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	7.09E+00	1.70E+00	4.18E+00	1.55E-03	3.35E+00	1.08E+01
ln(day)	-6.55E-01	3.38E-01	-1.94E+00	7.83E-02	-1.40E+00	8.77E-02

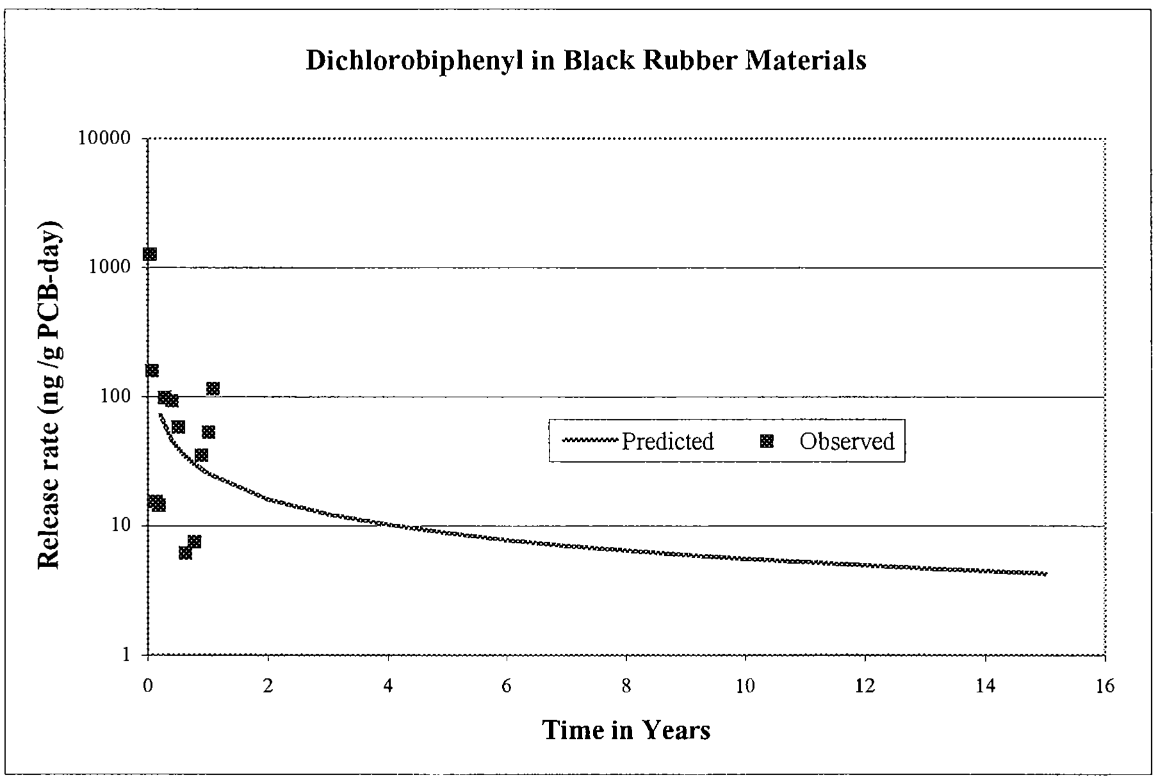
RESIDUAL OUTPUT

Observation	*cted ln(ng/g-PC*	*Residuals*
1	5.36E+00	1.79E+00
2	4.90E+00	1.57E-01
3	4.54E+00	-1.82E+00
4	4.31E+00	-1.66E+00
5	4.05E+00	5.30E-01
6	3.83E+00	6.90E-01
7	3.66E+00	3.85E-01
8	3.53E+00	-1.72E+00
9	3.38E+00	-1.38E+00
10	3.30E+00	2.53E-01

Observation	*dicted ln(ng/g-PCI*	*Residuals*
11	3.22E+00	7.40E-01
12	3.17E+00	1.57E+00
13	3.05E+00	4.65E-01



Dichlorobiphenyl in Black Rubber Materials
Release Rate (ng/ g PCB - day)
Time in Days
Predicted
Observed
10000
1000
100
10
1
0
100
200
300
400
500
600



Dichlorobiphenyl in Black Rubber Materials
Release rate (ng /g PCB-day)
Time in Years
Predicted
Observed
10000
1000
100
10
1
0
2
4
6
8
10
12
14
16

Trichlorobiphenyl in Bulkhead Insulation

ng/ g-PCB - d	Cl3
6.25E-03	0
1.17E+00	0
7.07E+00	211
1.41E+01	239
2.82E+01	143
4.92E+01	77.8
6.93E+01	114
1.04E+02	80.1
1.46E+02	101.1
1.88E+02	61.9
2.30E+02	216.1
2.86E+02	162.2
3.28E+02	32.8
3.70E+02	45.6
3.98E+02	86
4.75E+02	57.0

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
2.64E+00	1.41E+01	239	5.48E+00
3.34E+00	2.82E+01	143	4.97E+00
3.90E+00	4.92E+01	78	4.35E+00
4.24E+00	6.93E+01	114	4.74E+00
4.65E+00	1.04E+02	80	4.38E+00
4.98E+00	1.46E+02	101	4.62E+00
5.24E+00	1.88E+02	62	4.13E+00
5.44E+00	2.30E+02	216	5.38E+00
5.66E+00	2.86E+02	162	5.09E+00
5.79E+00	3.28E+02	33	3.49E+00
5.91E+00	3.70E+02	46	3.82E+00
5.99E+00	3.98E+02	86	4.45E+00
6.16E+00	4.75E+02	57	4.04E+00

Maximum Release Rate at 14 days
239 ng/gPCB-d

Release rate at 2 years
56.6 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.5534
R Square	0.3063
Standard Error	0.5150
Observations	13

ANOVA

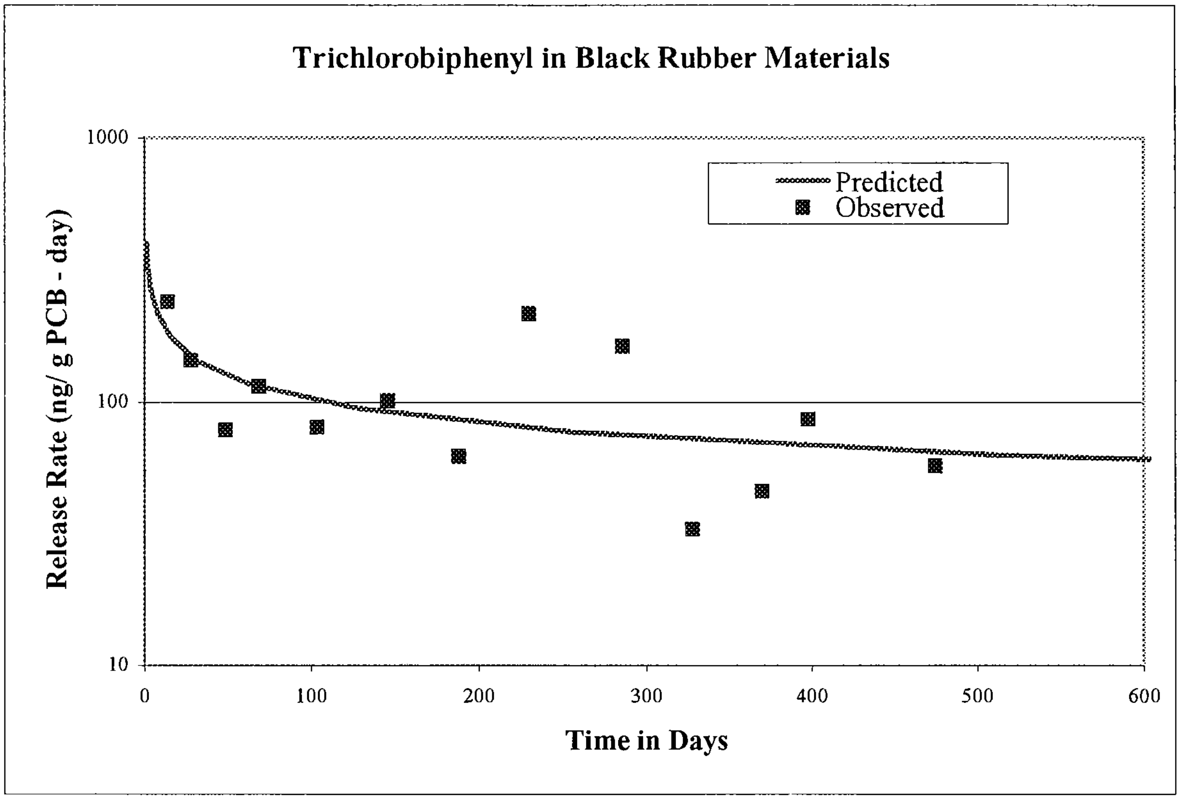
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.29E+00	1.29E+00	4.86E+00	4.98E-02
Residual	11	2.92E+00	2.65E-01		
Total	12	4.21E+00			

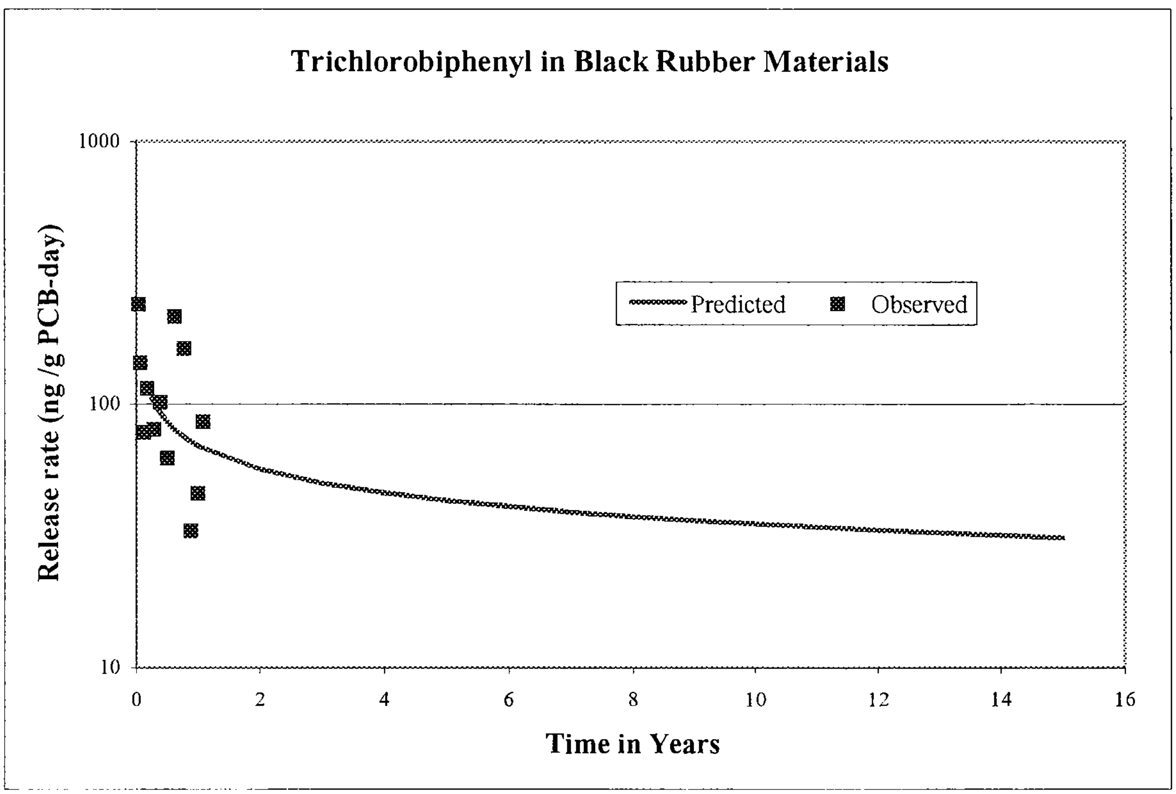
	Coefficients	*andard Erro*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	5.99E+00	6.78E-01	8.84E+00	2.49E-06	4.50E+00	7.48E+00
ln(day)	-2.97E-01	1.35E-01	-2.20E+00	4.98E-02	-5.93E-01	-3.71E-04

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	5.21E+00	2.69E-01
2	5.00E+00	-3.64E-02
3	4.84E+00	-4.83E-01
4	4.73E+00	3.60E-03
5	4.61E+00	-2.31E-01
6	4.51E+00	1.02E-01
7	4.44E+00	-3.13E-01
8	4.38E+00	9.97E-01
9	4.31E+00	7.75E-01
10	4.27E+00	-7.81E-01
11	4.24E+00	-4.17E-01

12	4.22E+00	2.35E-01
13	4.16E+00	-1.20E-01





Tetrachlorobiphenyl in Bulkhead Insulation

ng/ g-PCB - d	Cl4
6.25E-03	0
1.17E+00	0
7.07E+00	736
1.41E+01	922
2.82E+01	688
4.92E+01	654.5
6.93E+01	895
1.04E+02	486.2
1.46E+02	413.8
1.88E+02	295.1
2.30E+02	272.5
2.86E+02	137.5
3.28E+02	180.9
3.70E+02	204.3
3.98E+02	271
4.75E+02	163.3

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
2.64E+00	1.41E+01	922	6.83E+00
3.34E+00	2.82E+01	688	6.53E+00
3.90E+00	4.92E+01	654	6.48E+00
4.24E+00	6.93E+01	895	6.80E+00
4.65E+00	1.04E+02	486	6.19E+00
4.98E+00	1.46E+02	414	6.03E+00
5.24E+00	1.88E+02	295	5.69E+00
5.44E+00	2.30E+02	273	5.61E+00
5.66E+00	2.86E+02	137	4.92E+00
5.79E+00	3.28E+02	181	5.20E+00
5.91E+00	3.70E+02	204	5.32E+00
5.99E+00	3.98E+02	271	5.60E+00
6.16E+00	4.75E+02	163	5.10E+00

Maximum Release Rate at 14 days
922 ng/gPCB-d

Release rate at 2 years
144 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.9041
Adjusted R Squ	0.8007
Standard Error	0.2921
Observations	13

ANOVA

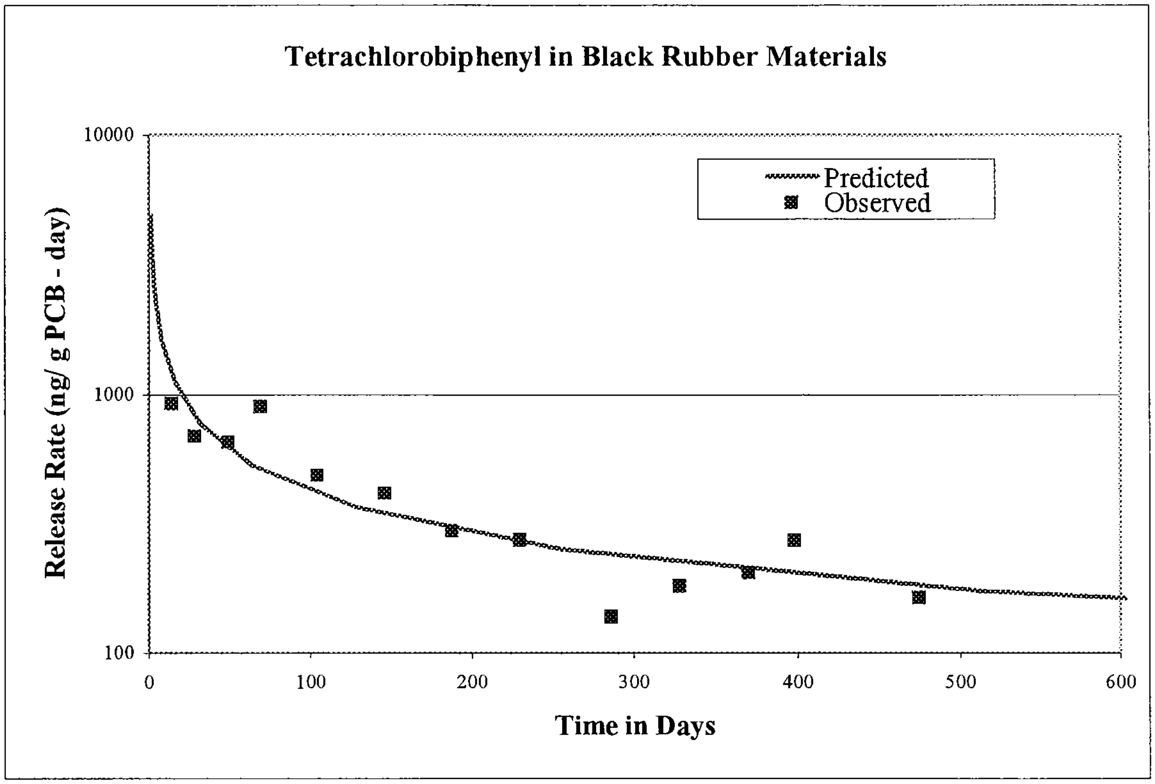
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	4.20E+00	4.20E+00	4.92E+01	2.22E-05
Residual	11	9.39E-01	8.53E-02		
Total	12	5.14E+00			

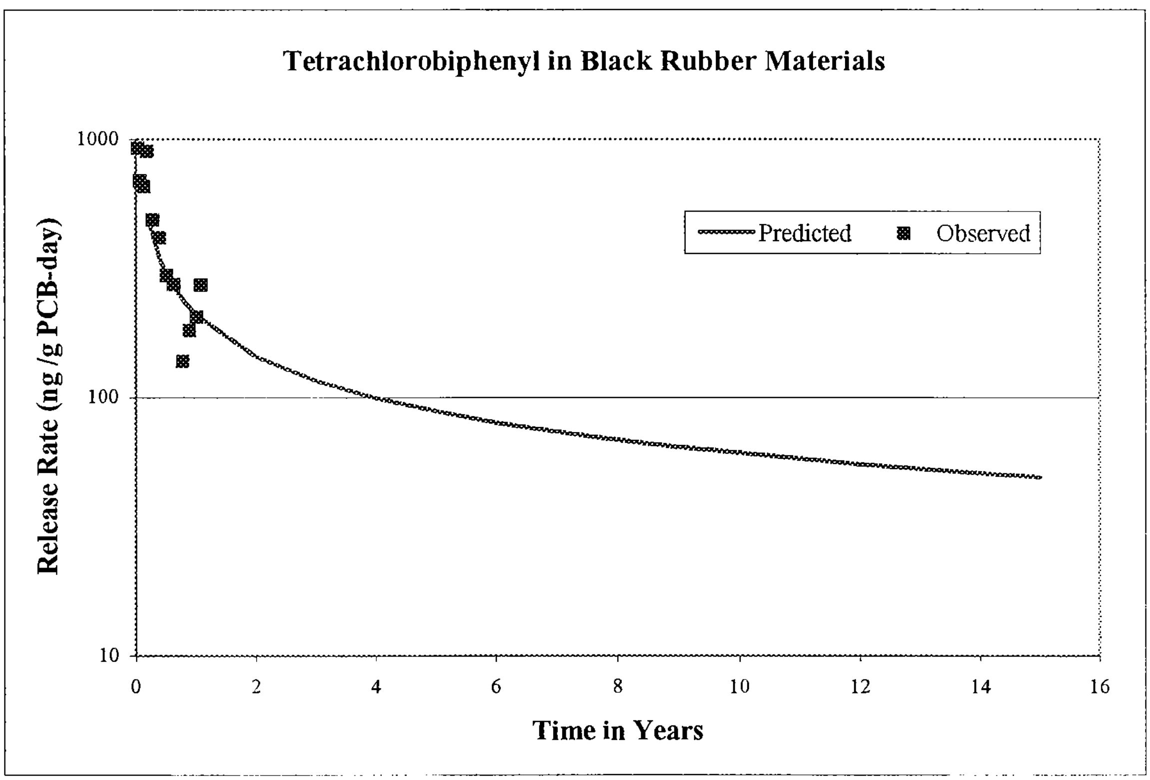
	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	8.50E+00	3.84E-01	2.21E+01	1.81E-10	7.66E+00	9.35E+00
ln(day)	-5.36E-01	7.64E-02	-7.02E+00	2.22E-05	-7.04E-01	-3.68E-01

RESIDUAL OUTPUT

Observation	*cted ln(ng/g-PC*	*Residuals*
1	7.09E+00	-2.61E-01
2	6.72E+00	-1.81E-01
3	6.42E+00	6.75E-02
4	6.23E+00	5.64E-01
5	6.01E+00	1.72E-01
6	5.83E+00	1.93E-01
7	5.70E+00	-1.02E-02
8	5.59E+00	1.84E-02
9	5.47E+00	-5.49E-01
10	5.40E+00	-2.01E-01

Observation	*licted ln(ng/g-PC*	*Residuals*
11	5.33E+00	-1.50E-02
12	5.30E+00	3.08E-01
13	5.20E+00	-1.05E-01


Tetrachlorobiphenyl in Black Rubber Materials
Predicted
Observed
Release Rate (ng/ g PCB - day)
10000
1000
100
0
100
200
300
400
500
600
Time in Days


Tetrachlorobiphenyl in Black Rubber Materials
Predicted
Observed
Release Rate (ng /g PCB-day)
1000
100
10
0
2
4
6
8
10
12
14
16
Time in Years

Pentachlorobiphenyl in Bulkhead Insulation

ng/ g-PCB - d	Cl5
6.25E-03	0
1.17E+00	0
7.07E+00	602
1.41E+01	461
2.82E+01	574
4.92E+01	379
6.93E+01	638
1.04E+02	458
1.46E+02	414
1.88E+02	248
2.30E+02	249
2.86E+02	53
3.28E+02	129
3.70E+02	109
3.98E+02	221
4.75E+02	111

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
4.24E+00	6.93E+01	638	6.46E+00
4.65E+00	1.04E+02	458	6.13E+00
4.98E+00	1.46E+02	414	6.03E+00
5.24E+00	1.88E+02	248	5.51E+00
5.44E+00	2.30E+02	249	5.52E+00
5.66E+00	2.86E+02	53	3.97E+00
5.79E+00	3.28E+02	129	4.86E+00
5.91E+00	3.70E+02	109	4.69E+00
5.99E+00	3.98E+02	221	5.40E+00
6.16E+00	4.75E+02	111	4.71E+00

Maximum Release Rate at 69 days
638 ng/gPCB-d

Release rate at 2 years
63.1 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.8104
R Square	0.6567
Standard Error	0.4781
Observations	10

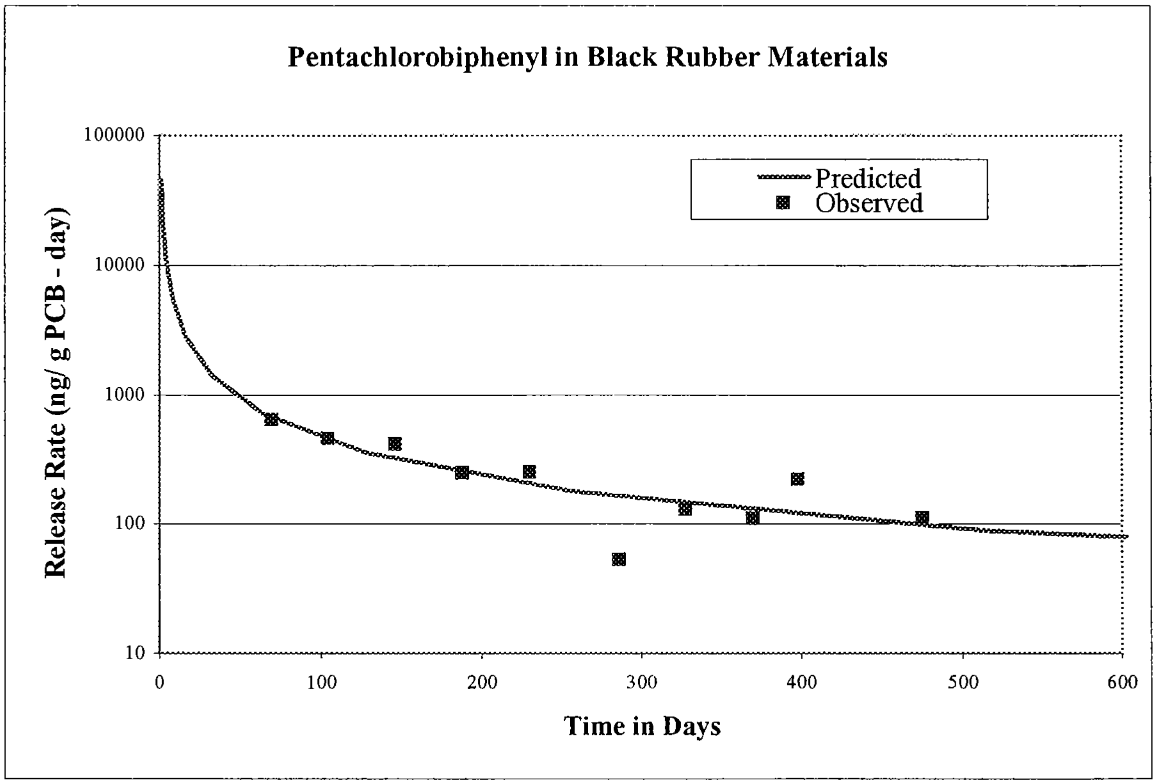
ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	3.50E+00	3.50E+00	1.53E+01	4.47E-03
Residual	8	1.83E+00	2.29E-01		
Total	9	5.33E+00			

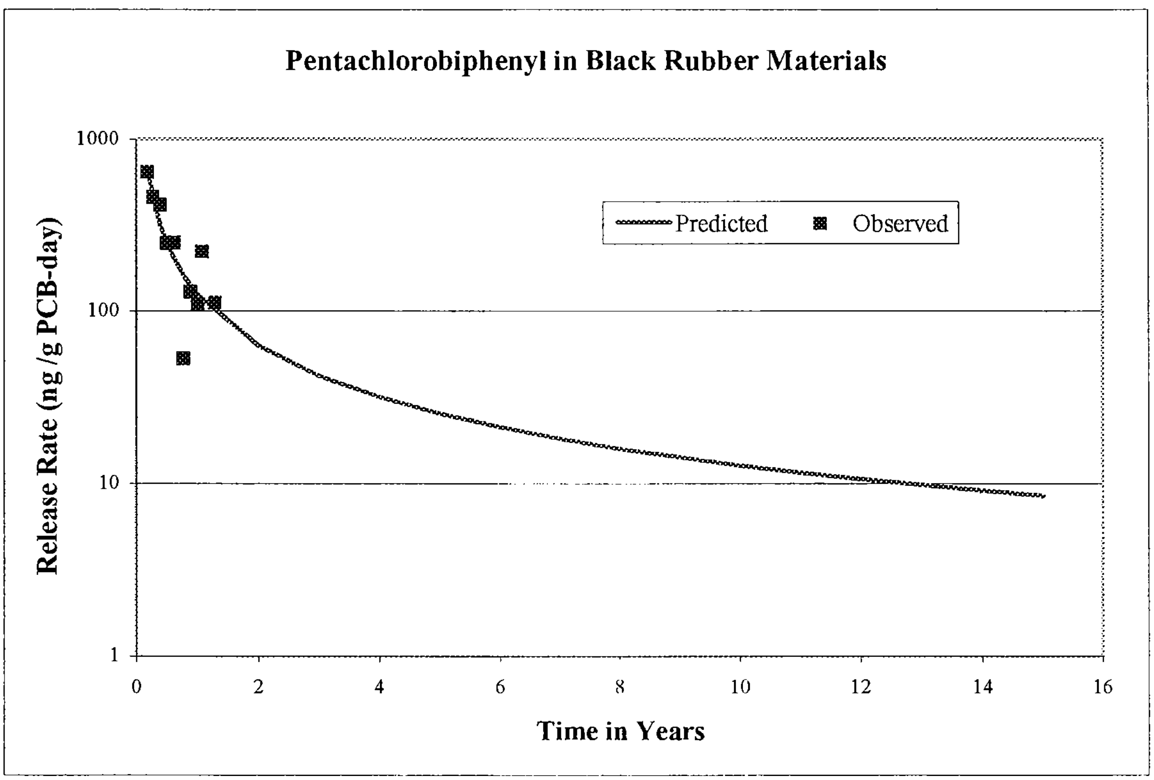
	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	1.07E+01	1.38E+00	7.74E+00	5.54E-05	7.52E+00	1.39E+01
ln(day)	-9.95E-01	2.54E-01	-3.91E+00	4.47E-03	-1.58E+00	-4.09E-01

RESIDUAL OUTPUT

Observation	*cted ln(ng/g-PC*	*Residuals*
1	6.49E+00	-3.12E-02
2	6.08E+00	4.27E-02
3	5.75E+00	2.79E-01
4	5.50E+00	1.63E-02
5	5.29E+00	2.23E-01
6	5.08E+00	-1.11E+00
7	4.94E+00	-8.50E-02
8	4.82E+00	-1.27E-01
9	4.75E+00	6.51E-01
10	4.57E+00	1.41E-01



Pentachlorobiphenyl in Black Rubber Materials
Predicted
Observed
100000
10000
1000
100
10
Release Rate (ng/ g PCB - day)
0
100
200
300
400
500
600
Time in Days



Pentachlorobiphenyl in Black Rubber Materials
Predicted
Observed
1000
100
10
1
Release Rate (ng /g PCB-day)
0
2
4
6
8
10
12
14
16
Time in Years

Heptachlorobiphenyl in Bulkhead Insulation

ng/ g-PCB - d	Cl7
6.25E-03	167503
1.17E+00	833
7.07E+00	311
1.41E+01	222
2.82E+01	0
4.92E+01	0
6.93E+01	0
1.04E+02	0
1.46E+02	0
1.88E+02	0
2.30E+02	0
2.86E+02	0
3.28E+02	0
3.70E+02	0
3.98E+02	0
4.75E+02	0

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
-5.08E+00	6.25E-03	167503	1.20E+01
1.56E-01	1.17E+00	833	6.72E+00
1.96E+00	7.07E+00	311	5.74E+00
2.64E+00	1.41E+01	222	5.40E+00

Maximum Release Rate at less than 1 day
167503 ng/gPCB-d

Release rate at 2 years
5.04 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.9925
R Square	0.9850
Standard Error	0.4626
Observations	4

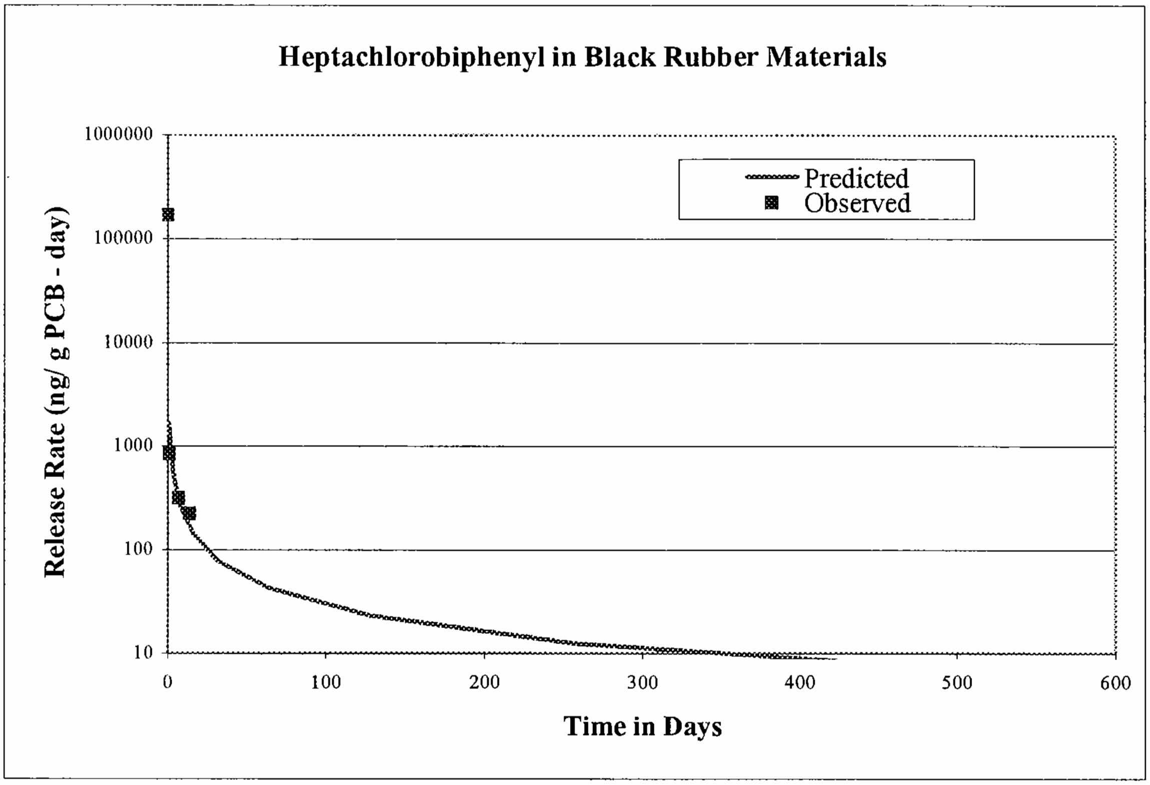
ANOVA

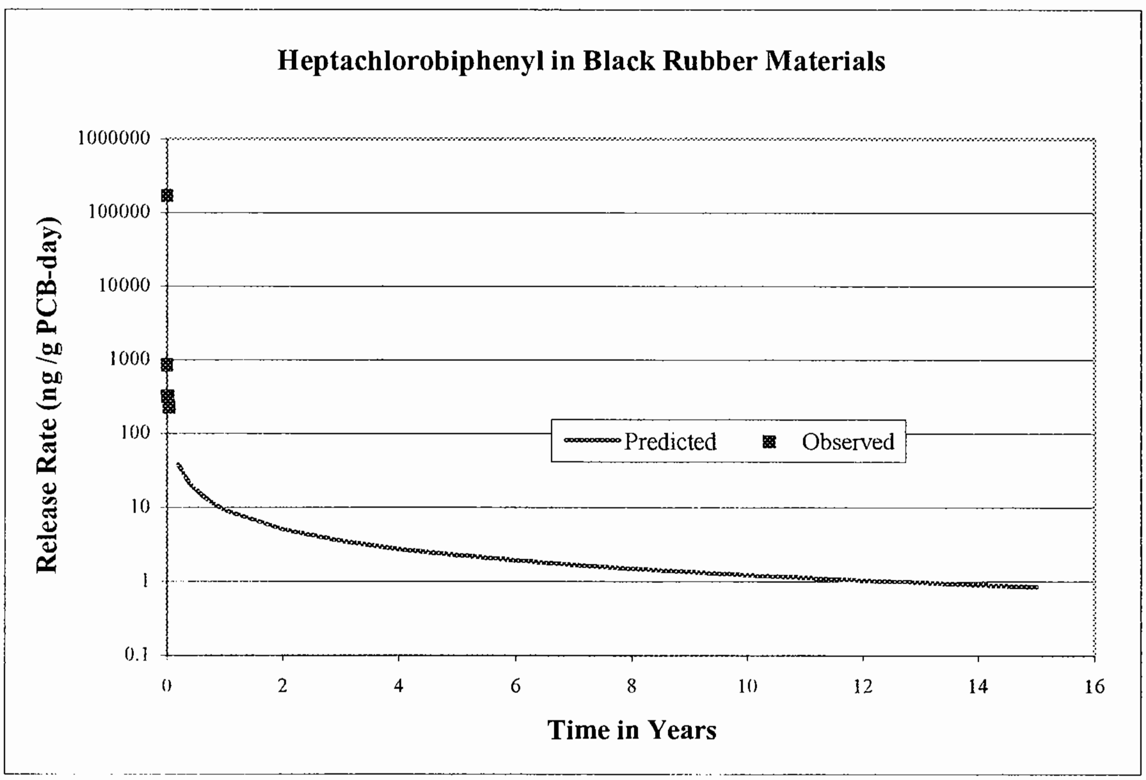
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	2.82E+01	2.82E+01	1.32E+02	7.51E-03
Residual	2	4.28E-01	2.14E-01		
Total	3	2.86E+01			

	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	7.40E+00	2.31E-01	3.20E+01	9.75E-04	6.41E+00	8.40E+00
ln(day)	-8.78E-01	7.65E-02	-1.15E+01	7.51E-03	-1.21E+00	-5.49E-01

RESIDUAL OUTPUT

Observation	*cted ln(ng/g-PC*	*Residuals*
1	1.19E+01	1.70E-01
2	7.27E+00	-5.43E-01
3	5.69E+00	5.33E-02
4	5.08E+00	3.19E-01


Heptachlorobiphenyl in Black Rubber Materials
Predicted
Observed
Release Rate (ng/ g PCB - day)
1000000
100000
10000
1000
100
10
0
100
200
300
400
500
600
Time in Days


Heptachlorobiphenyl in Black Rubber Materials
Predicted
Observed
Release Rate (ng /g PCB-day)
1000000
100000
10000
1000
100
10
1
0.1
0
2
4
6
8
10
12
14
16
Time in Years

BULKHEAD INSULATION

Bulkhead Insulation

Leaching Time (days)	Homologue Leach Rates (ng PCB/g shipboard solid-day)									
	Cl1	Cl2	Cl3	Cl4	Cl5	Cl6	Cl7	Cl8	Cl9	Cl10
6.94E-03	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
1.17E+00	0.0E+00	0.0E+00	1.2E+00	2.7E+01	2.6E+01	0.0E+00	1.5E+01	0.0E+00	0.0E+00	0.0E+00
7.08E+00	0.0E+00	2.6E+00	3.6E+00	4.5E+01	4.2E+01	7.0E+00	2.6E+00	0.0E+00	0.0E+00	0.0E+00
1.41E+01	0.0E+00	3.6E+00	3.1E+00	5.9E+01	6.4E+01	7.2E+00	1.6E+00	0.0E+00	0.0E+00	0.0E+00
2.11E+01	0.0E+00	1.8E-01	2.8E+00	7.0E+01	1.3E+02	1.9E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00
4.22E+01	0.0E+00	8.6E-02	1.5E+00	3.3E+01	4.9E+01	7.6E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
6.93E+01	0.0E+00	6.1E-02	1.3E+00	4.3E+01	1.0E+02	2.3E+01	0.0E+00	0.0E+00	0.0E+00	0.0E+00
8.31E+01	0.0E+00	0.0E+00	1.6E+00	4.7E+01	1.2E+02	2.1E+01	1.9E+00	0.0E+00	0.0E+00	0.0E+00
1.18E+02	0.0E+00	4.0E-02	9.2E-01	2.4E+01	4.5E+01	9.2E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
1.67E+02	0.0E+00	2.7E-02	6.5E-01	3.1E+01	8.7E+01	2.2E+01	1.6E+00	0.0E+00	0.0E+00	0.0E+00
2.09E+02	0.0E+00	2.2E-02	6.0E-01	1.7E+01	3.5E+01	8.1E+00	8.1E-01	0.0E+00	0.0E+00	0.0E+00
2.51E+02	0.0E+00	0.0E+00	6.7E-01	2.0E+01	4.2E+01	8.4E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
2.86E+02	0.0E+00	0.0E+00	5.1E-01	1.7E+01	2.5E+01	3.9E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
3.28E+02	0.0E+00	0.0E+00	5.1E-01	1.2E+01	2.4E+01	5.9E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
3.70E+02	0.0E+00	0.0E+00	5.5E-01	1.4E+01	2.1E+01	4.2E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
3.98E+02	0.0E+00	0.0E+00	1.1E+00	1.7E+01	2.9E+01	8.3E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
4.54E+02	0.0E+00	0.0E+00	6.0E-01	7.3E+00	1.2E+01	4.1E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
Max	0.0E+00	3.6E+00	3.6E+00	7.0E+01	1.3E+02	2.3E+01	1.5E+01	0.0E+00	0.0E+00	0.0E+00
Min	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00

0.00044 g PCB / g bulkhead insulation (leachate study concentration)

Leaching Time (days)	Homologue Leach Rates (ng PCB/g PCB-day)									
ng/ g-PCB - d	Cl1	Cl2	Cl3	Cl4	Cl5	Cl6	Cl7	Cl8	Cl9	Cl10
0.007	0	0	0	0	0	0	0	0	0	0
1.170	0	0	2662	62223	58766	0	34568	0	0	0
7.076	0	5988	8259	103242	96359	15830	5919	0	0	0
14.083	0	8209	7036	134856	146583	16417	3694	0	0	0
21.097	0	398	6443	158137	286990	42170	0	0	0	0
42.226	0	194	3306	73888	110832	17305	0	0	0	0
69.301	0	138	2873	97698	229878	53159	0	0	0	0
83.139	0	0	3525	105743	267294	46997	4406	0	0	0
118.135	0	92	2091	53427	103369	20906	0	0	0	0
167.104	0	62	1478	71438	197072	50089	3695	0	0	0
209.131	0	50	1354	38687	79308	18376	1838	0	0	0
251.192	0	0	1530	45887	95598	19120	0	0	0	0
286.150	0	0	1150	39107	56361	8972	0	0	0	0
328.092	0	0	1150	26843	55604	13422	0	0	0	0
370.117	0	0	1244	31575	47841	9568	0	0	0	0
398.079	0	0	2471	37794	66867	18897	0	0	0	0
454.319	0	0	1373	16623	28187	9396	0	0	0	0
Max	0	8209	8259	158137	286990	53159	34568	0	0	0
Min	0	0	0	0	0	0	0	0	0	0
Median	0	0	2091	53427	95598	17305	0	0	0	0
Simple Average	0	890	2820	64539	113348	21213	3184	0	0	0
Number of detects	0	8	16	16	16	15	6	0	0	0
Number of nondetects	17	9	1	1	1	2	11	17	17	17
Intercept	---	1.16E+01	1.00E+01	1.38E+01	1.46E+01	1.45E+01	9.97E+00	---	---	---
Slope	---	-1.50E+00	-4.85E-01	-5.89E-01	-6.21E-01	-8.69E-01	-4.24E-01	---	---	---
alpha	---	7.11E-03	4.14E-07	2.63E-05	6.54E-04	1.37E-03	2.43E-02	---	---	---

Dichlorobiphenyl in Bulkhead Insulation

ng/ g-PCB - d	Cl2
6.94E-03	0
1.17E+00	0
7.08E+00	5988
1.41E+01	8209
2.11E+01	398
4.22E+01	194
6.93E+01	138
8.31E+01	0
1.18E+02	92
1.67E+02	62
2.09E+02	50
2.51E+02	0
2.86E+02	0
3.28E+02	0
3.70E+02	0
3.98E+02	0
4.54E+02	0

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
2.64E+00	1.41E+01	8209	9.013E+00
3.05E+00	2.11E+01	398	5.987E+00
3.74E+00	4.22E+01	194	5.270E+00
4.24E+00	6.93E+01	138	4.927E+00
4.77E+00	1.18E+02	92	4.519E+00
5.12E+00	1.67E+02	62	4.134E+00
5.34E+00	2.09E+02	50	3.918E+00

Maximum Release Rate at 7 day
8209 ng/gPCB-d

Release rate at 2 years
5.43 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.8909
R Square	0.7938
Standard Error	0.8668
Observations	7

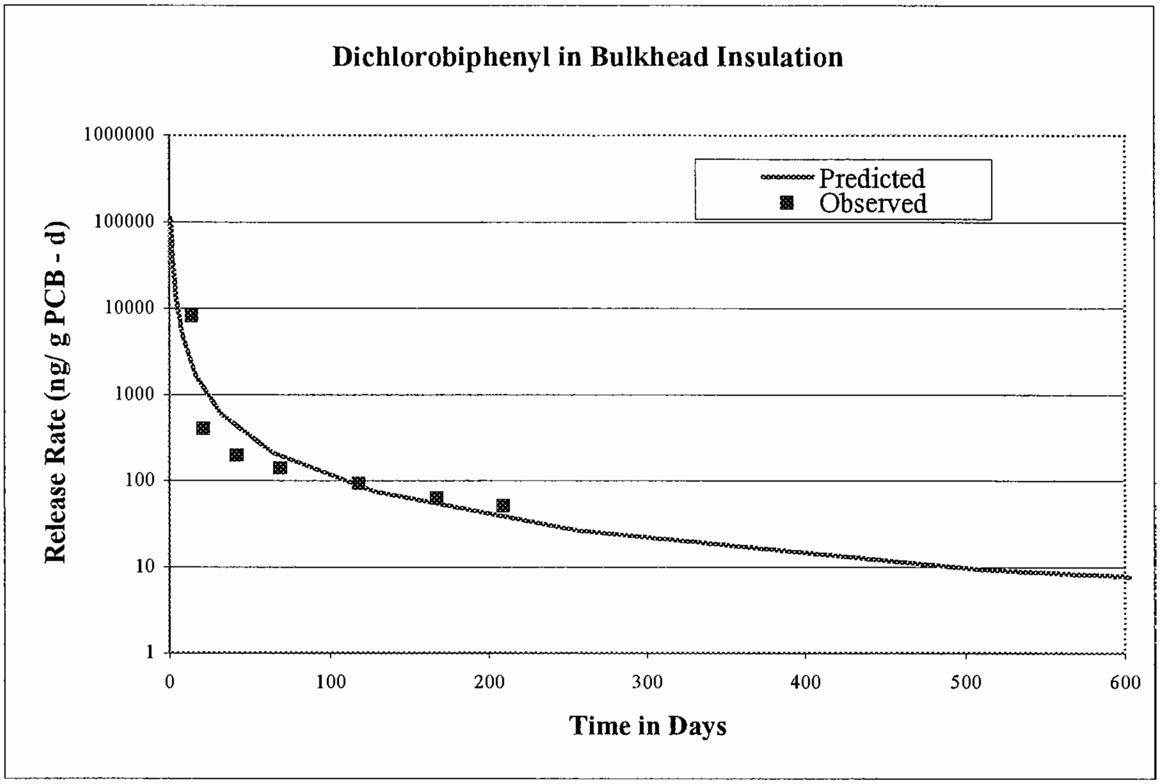
ANOVA

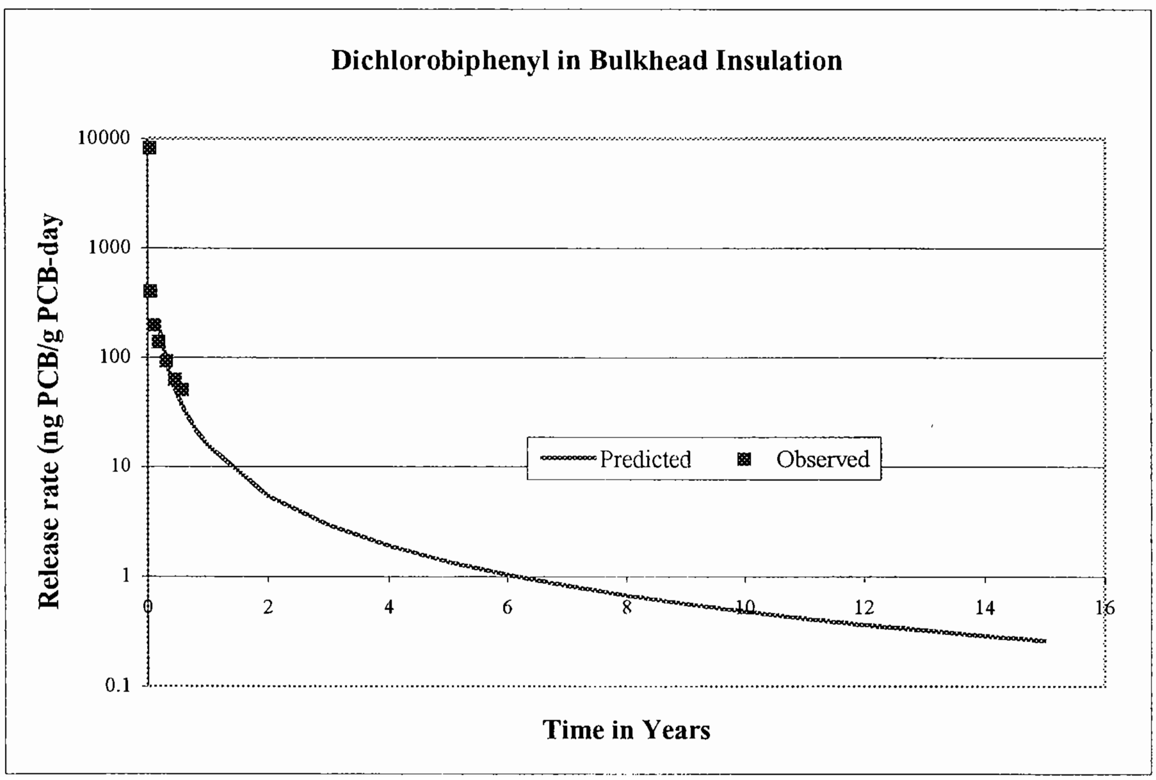
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.45E+01	1.45E+01	1.92E+01	7.11E-03
Residual	5	3.76E+00	7.51E-01		
Total	6	1.82E+01			

	Coefficients	*Std Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	1.16E+01	1.45E+00	7.99E+00	4.97E-04	7.87E+00	1.53E+01
ln(day)	-1.50E+00	3.43E-01	-4.39E+00	7.11E-03	-2.38E+00	-6.22E-01

RESIDUAL OUTPUT

Observation	*cted ln(ng/g-PC*	*Residuals*
1	7.63E+00	1.38E+00
2	7.02E+00	-1.03E+00
3	5.98E+00	-7.07E-01
4	5.23E+00	-3.05E-01
5	4.43E+00	8.90E-02
6	3.91E+00	2.25E-01
7	3.57E+00	3.46E-01


Dichlorobiphenyl in Bulkhead Insulation
Predicted
Observed
Release Rate (ng/ g PCB - d)
1000000
100000
10000
1000
100
10
1
0
100
200
300
400
500
600
Time in Days


Dichlorobiphenyl in Bulkhead Insulation
Predicted
Observed
Release rate (ng PCB/g PCB-day
10000
1000
100
10
1
0.1
0
2
4
6
8
10
12
14
16
Time in Years

Trichlorobiphenyl in Bulkhead Insulation

ng/ g-PCB - d	C13
6.94E-03	0
1.17E+00	2662
7.08E+00	8259
1.41E+01	7036
2.11E+01	6443
4.22E+01	3306
6.93E+01	2873
8.31E+01	3525
1.18E+02	2091
1.67E+02	1478
2.09E+02	1354
2.51E+02	1530
2.86E+02	1150
3.28E+02	1150
3.70E+02	1244
3.98E+02	2471
4.54E+02	1373

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
1.96E+00	7.08E+00	8259	9.02E+00
2.64E+00	1.41E+01	7036	8.86E+00
3.05E+00	2.11E+01	6443	8.77E+00
3.74E+00	4.22E+01	3306	8.10E+00
4.24E+00	6.93E+01	2873	7.96E+00
4.42E+00	8.31E+01	3525	8.17E+00
4.77E+00	1.18E+02	2091	7.65E+00
5.12E+00	1.67E+02	1478	7.30E+00
5.34E+00	2.09E+02	1354	7.21E+00
5.53E+00	2.51E+02	1530	7.33E+00
5.66E+00	2.86E+02	1150	7.05E+00
5.79E+00	3.28E+02	1150	7.05E+00
5.91E+00	3.70E+02	1244	7.13E+00
5.99E+00	3.98E+02	2471	7.81E+00
6.12E+00	4.54E+02	1373	7.22E+00

Maximum Release Rate at 7 day
8259 ng/gPCB-d

Release rate at 2 years
944 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.9324
Adjusted R Squ	0.8593
Standard Error	0.2566
Observations	15

ANOVA

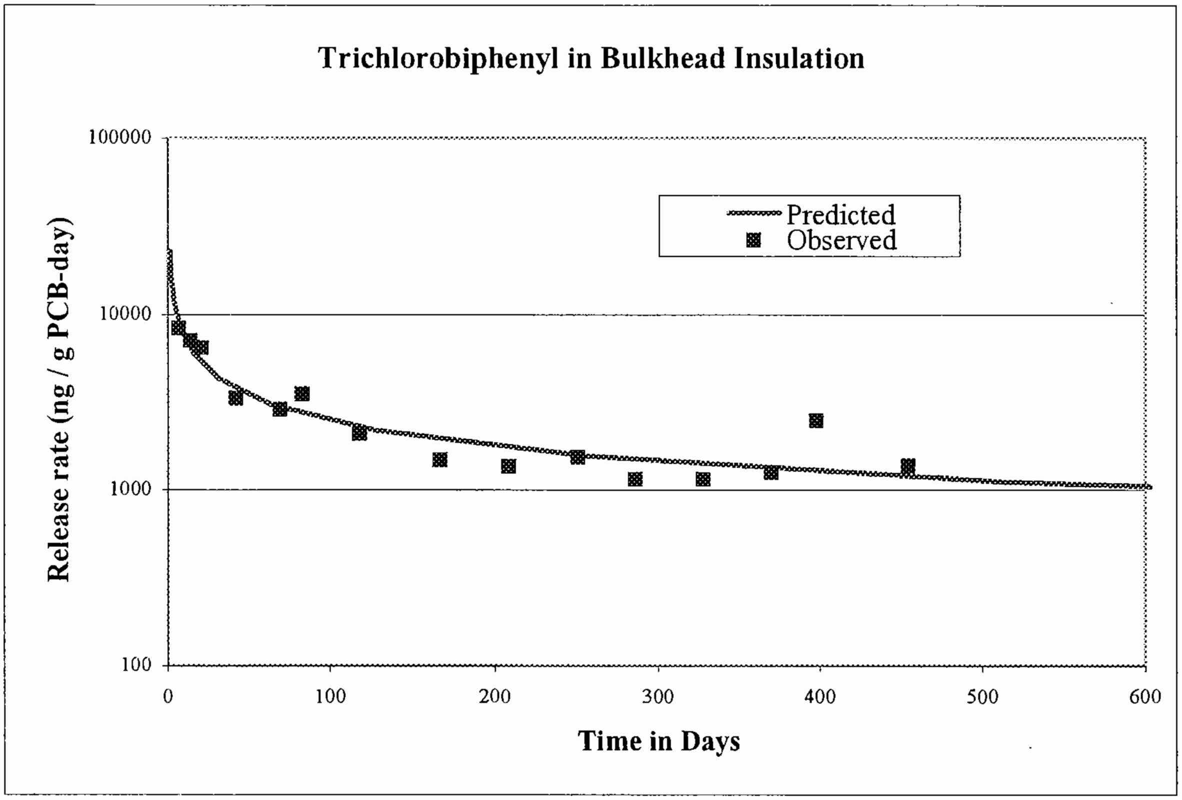
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	5.70E+00	5.70E+00	8.65E+01	4.14E-07
Residual	13	8.56E-01	6.58E-02		
Total	14	6.55E+00			

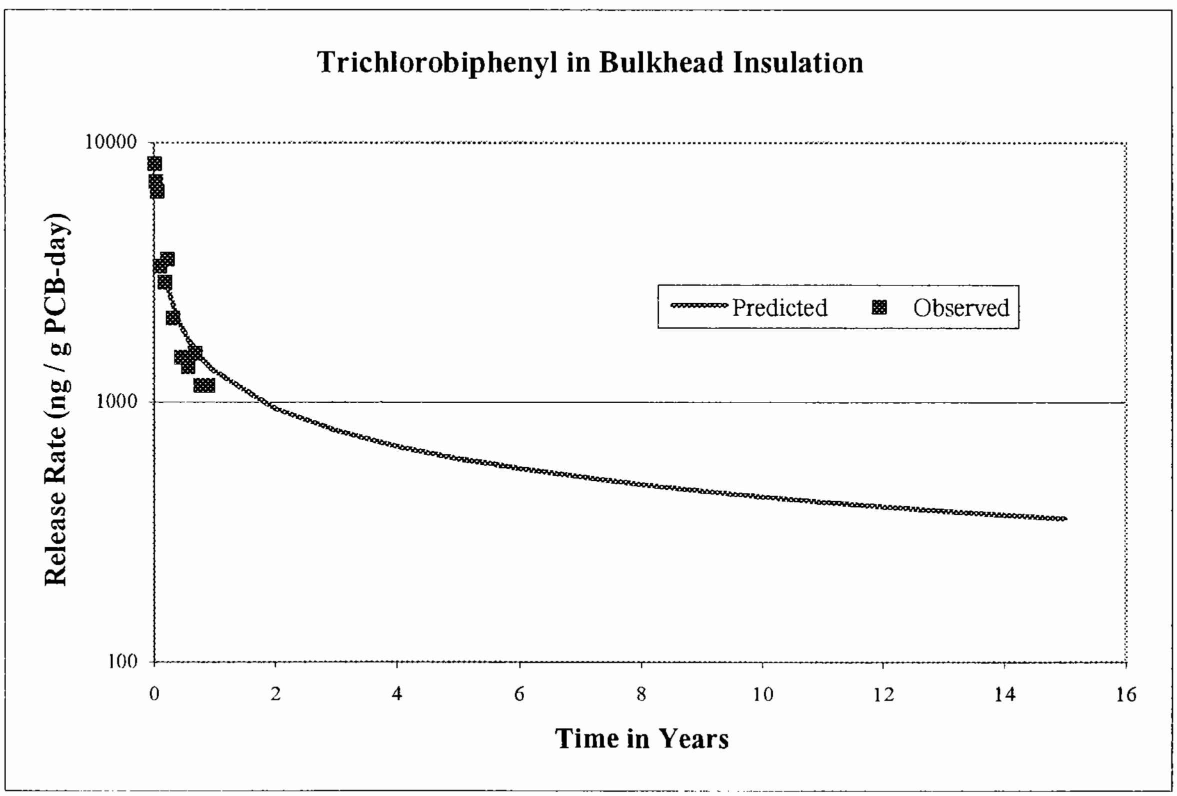
	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	1.00E+01	2.53E-01	3.97E+01	5.92E-15	9.50E+00	1.06E+01
ln(day)	-4.85E-01	5.21E-02	-9.30E+00	4.14E-07	-5.98E-01	-3.72E-01

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	9.10E+00	-7.99E-02
2	8.77E+00	9.37E-02
3	8.57E+00	2.02E-01
4	8.23E+00	-1.29E-01
5	7.99E+00	-2.88E-02
6	7.90E+00	2.64E-01
7	7.73E+00	-8.81E-02
8	7.57E+00	-2.67E-01
9	7.46E+00	-2.45E-01
10	7.37E+00	-3.47E-02

Observatiordicted ln(ng/g-PC1		*Residuals*
11	7.30E+00	-2.56E-01
12	7.24E+00	-1.90E-01
13	7.18E+00	-5.34E-02
14	7.14E+00	6.68E-01
15	7.08E+00	1.45E-01


Trichlorobiphenyl in Bulkhead Insulation
Predicted
Observed
100000
10000
1000
100
0
100
200
300
400
500
600
Release rate (ng / g PCB-day)
Time in Days


Trichlorobiphenyl in Bulkhead Insulation
Predicted
Observed
10000
1000
100
0
2
4
6
8
10
12
14
16
Release Rate (ng / g PCB-day)
Time in Years

Tetrachlorobiphenyl in Bulkhead Insulation

ng/ g-PCB - d	Cl4
6.94E-03	0
1.17E+00	62223
7.08E+00	103242
1.41E+01	134856
2.11E+01	158137
4.22E+01	73888
6.93E+01	97698
8.31E+01	105743
1.18E+02	53427
1.67E+02	71438
2.09E+02	38687
2.51E+02	45887
2.86E+02	39107
3.28E+02	26843
3.70E+02	31575
3.98E+02	37794
4.54E+02	16623

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
3.05E+00	2.11E+01	158137	1.20E+01
3.74E+00	4.22E+01	73888	1.12E+01
4.24E+00	6.93E+01	97698	1.15E+01
4.42E+00	8.31E+01	105743	1.16E+01
4.77E+00	1.18E+02	53427	1.09E+01
5.12E+00	1.67E+02	71438	1.12E+01
5.34E+00	2.09E+02	38687	1.06E+01
5.53E+00	2.51E+02	45887	1.07E+01
5.66E+00	2.86E+02	39107	1.06E+01
5.79E+00	3.28E+02	26843	1.02E+01
5.91E+00	3.70E+02	31575	1.04E+01
5.99E+00	3.98E+02	37794	1.05E+01
6.12E+00	4.54E+02	16623	9.72E+00

Maximum Release Rate at 21 days
158137 ng/gPCB-d

Release rate at 2 years
20704 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.9010
R Square	0.8117
Standard Error	0.2816
Observations	13

ANOVA

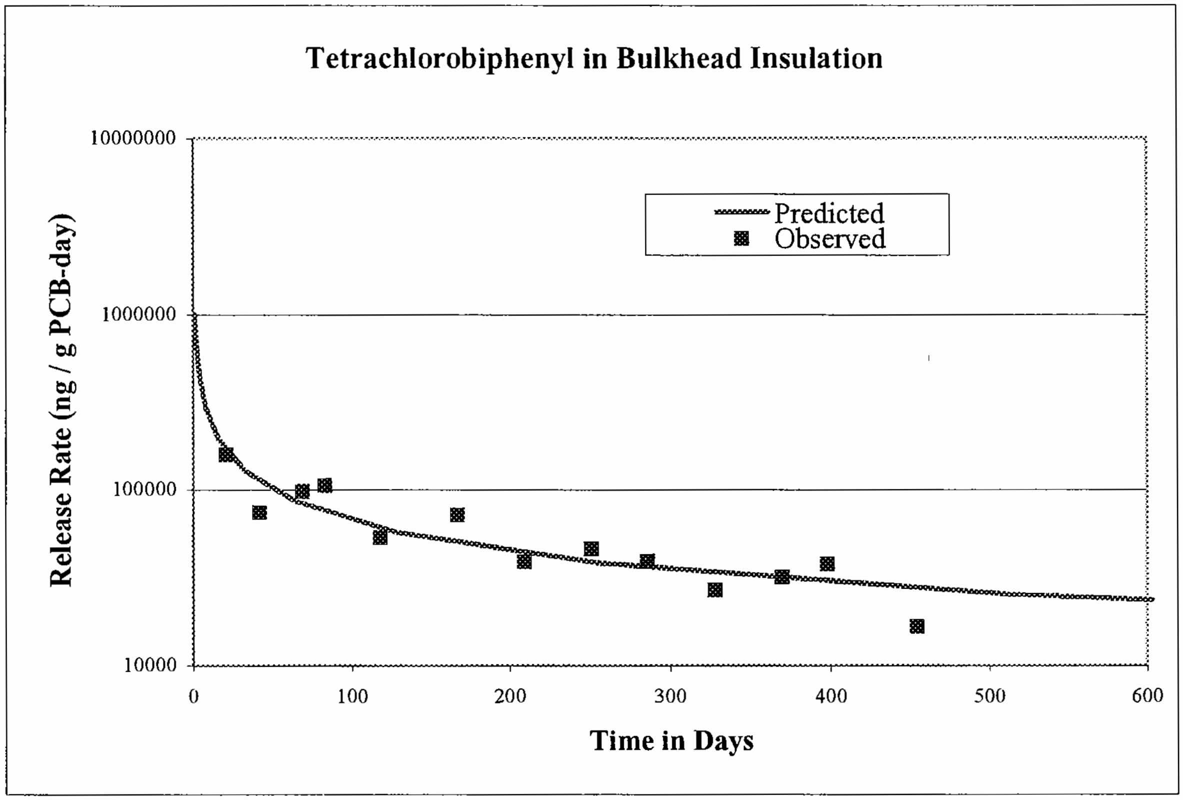
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	3.76E+00	3.76E+00	4.74E+01	2.63E-05
Residual	11	8.72E-01	7.93E-02		
Total	12	4.63E+00			

	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	1.38E+01	4.39E-01	3.15E+01	3.95E-12	1.29E+01	1.48E+01
ln(day)	-5.89E-01	8.55E-02	-6.89E+00	2.63E-05	-7.77E-01	-4.01E-01

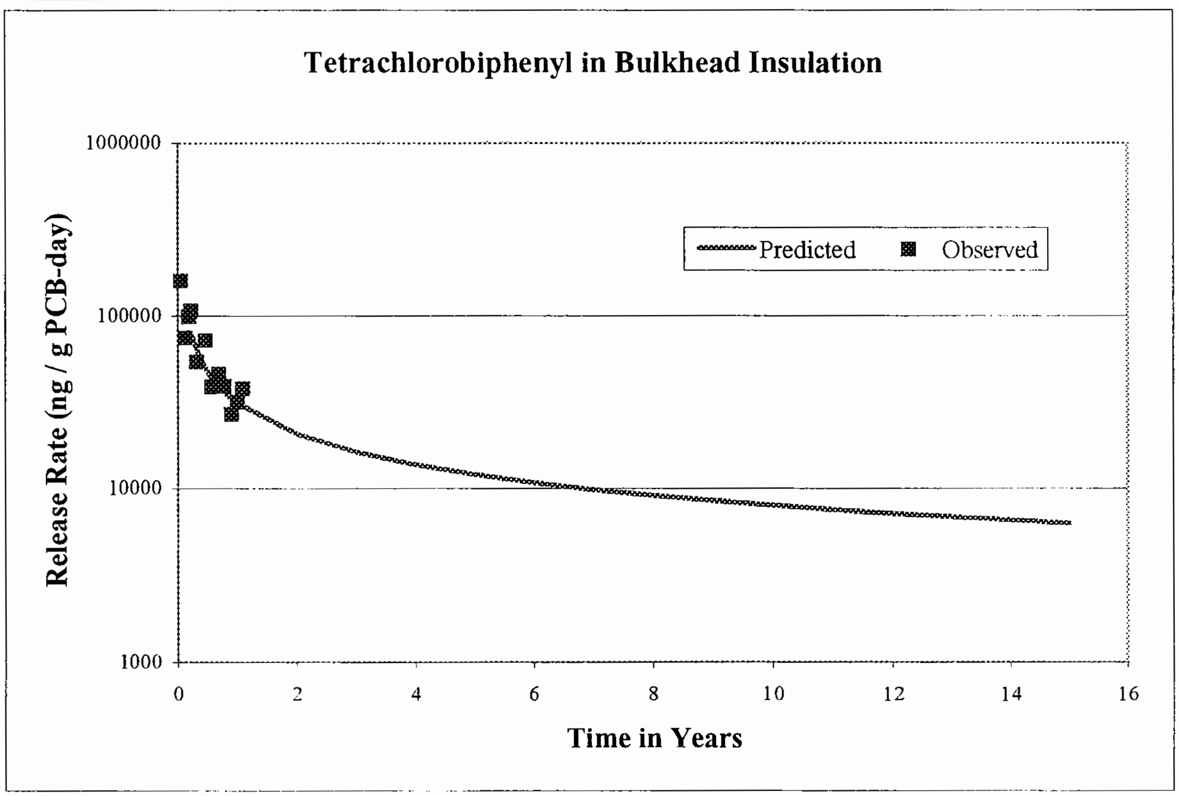
RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	1.20E+01	-5.38E-02
2	1.16E+01	-4.06E-01
3	1.13E+01	1.65E-01
4	1.12E+01	3.51E-01
5	1.10E+01	-1.24E-01
6	1.08E+01	3.70E-01
7	1.07E+01	-1.11E-01
8	1.06E+01	1.68E-01
9	1.05E+01	8.45E-02
10	1.04E+01	-2.11E-01

Observatiordicted ln(ng/g-PC1		*Residuals*
11	1.03E+01	2.21E-02
12	1.03E+01	2.45E-01
13	1.02E+01	-4.99E-01



Tetrachlorobiphenyl in Bulkhead Insulation
Predicted
Observed
Release Rate (ng / g PCB-day)
10000000
1000000
100000
10000
0
100
200
300
400
500
600
Time in Days



Tetrachlorobiphenyl in Bulkhead Insulation
Predicted
Observed
Release Rate (ng / g PCB-day)
1000000
100000
10000
1000
0
2
4
6
8
10
12
14
16
Time in Years

Pentachlorobiphenyl in Bulkhead Insulation

ng/ g-PCB - d	Cl5
0.007	0
1.170	58766
7.076	96359
14.083	146583
21.097	286990
42.226	110832
69.301	229878
83.139	267294
118.135	103369
167.104	197072
209.131	79308
251.192	95598
286.150	56361
328.092	55604
370.117	47841
398.079	66867
454.319	28187

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
3.05E+00	21.097	286990	1.26E+01
3.74E+00	42.226	110832	1.16E+01
4.24E+00	69.301	229878	1.23E+01
4.42E+00	83.139	267294	1.25E+01
4.77E+00	118.135	103369	1.15E+01
5.12E+00	167.104	197072	1.22E+01
5.34E+00	209.131	79308	1.13E+01
5.53E+00	251.192	95598	1.15E+01
5.66E+00	286.150	56361	1.09E+01
5.79E+00	328.092	55604	1.09E+01
5.91E+00	370.117	47841	1.08E+01
5.99E+00	398.079	66867	1.11E+01
6.12E+00	454.319	28187	1.02E+01

Maximum Release Rate at 21 days
286990 ng/gPCB-d

Release rate at 2 years
37917 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.8168
R Square	0.6672
Standard Error	0.4358
Observations	13

ANOVA

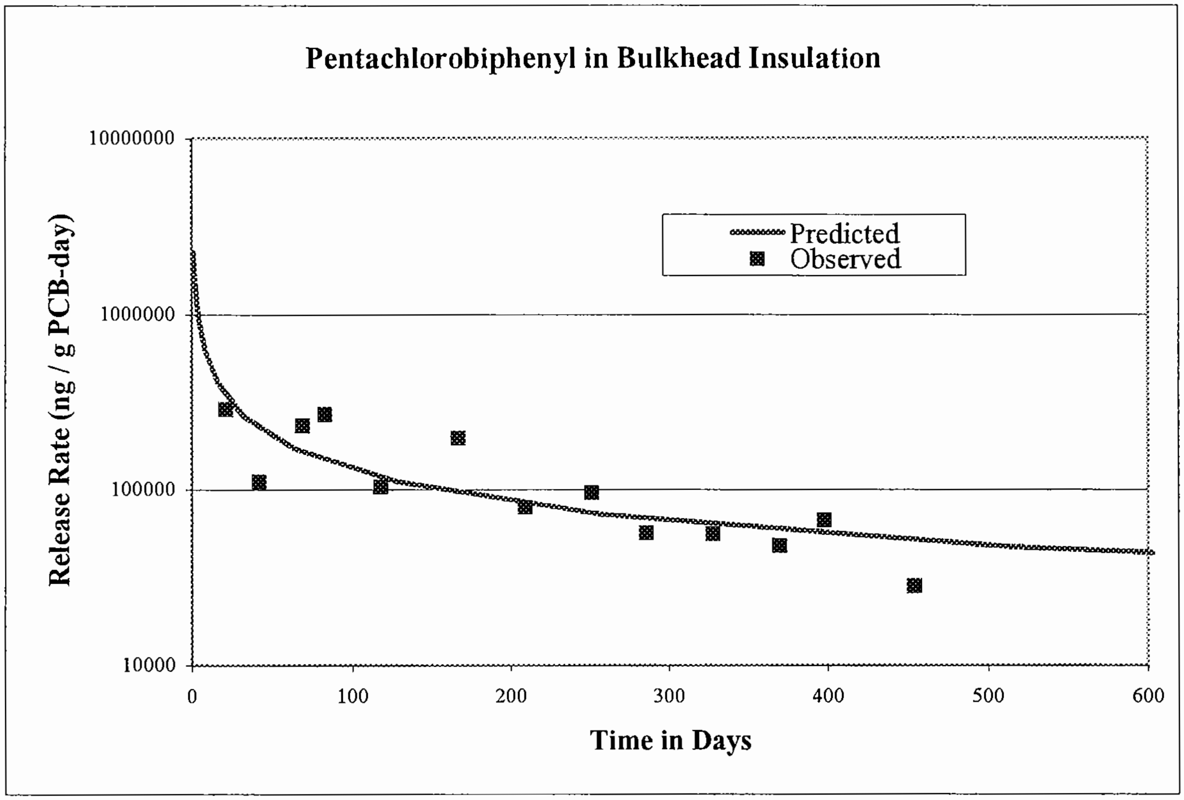
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	4.19E+00	4.19E+00	2.21E+01	6.54E-04
Residual	11	2.09E+00	1.90E-01		
Total	12	6.28E+00			

	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	1.46E+01	6.79E-01	2.15E+01	2.40E-10	1.31E+01	1.61E+01
ln(day)	-6.21E-01	1.32E-01	-4.70E+00	6.54E-04	-9.13E-01	-3.30E-01

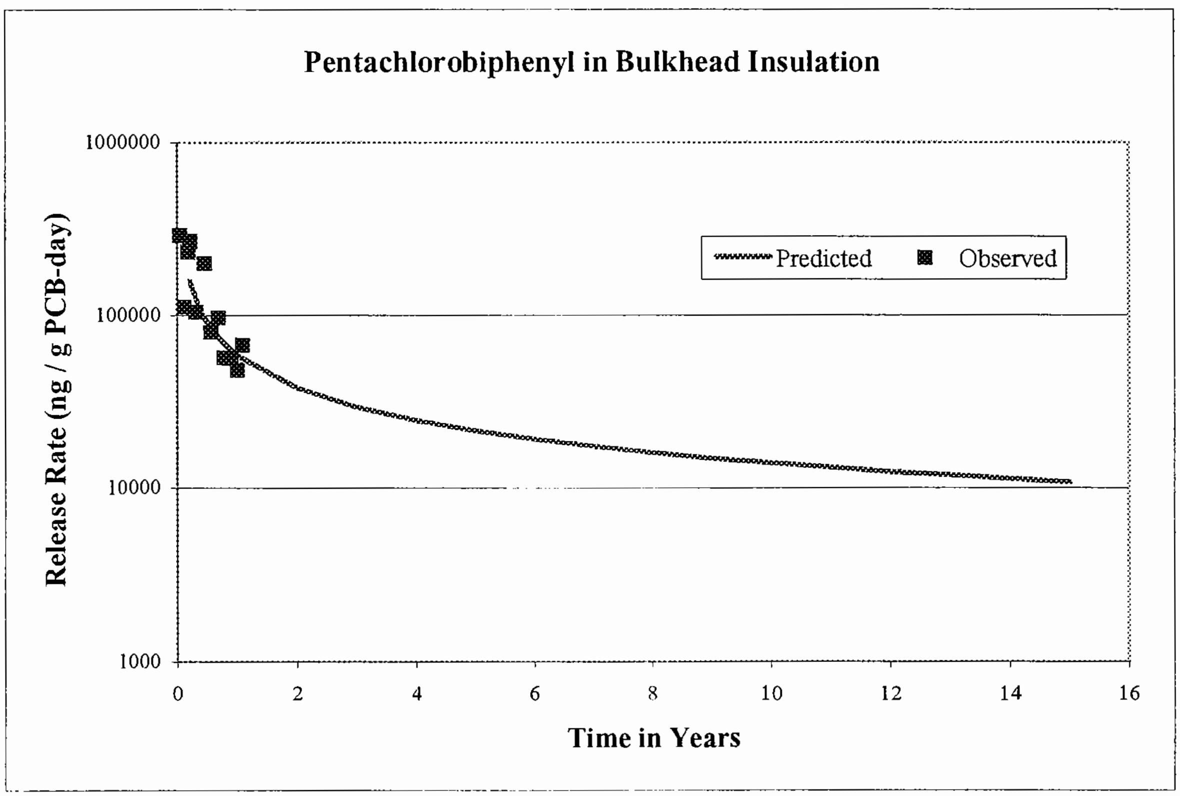
RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	1.27E+01	-1.78E-01
2	1.23E+01	-6.99E-01
3	1.20E+01	3.39E-01
4	1.19E+01	6.03E-01
5	1.17E+01	-1.29E-01
6	1.15E+01	7.32E-01
7	1.13E+01	-3.90E-02
8	1.12E+01	2.62E-01
9	1.11E+01	-1.86E-01
10	1.10E+01	-1.14E-01

Observatiodicted ln(ng/g-PC1		*Residuals*
11	1.10E+01	-1.90E-01
12	1.09E+01	1.90E-01
13	1.08E+01	-5.91E-01



Pentachlorobiphenyl in Bulkhead Insulation
Release Rate (ng / g PCB-day)
10000000
1000000
100000
10000
0
100
200
300
400
500
600
Time in Days
Predicted
Observed



Pentachlorobiphenyl in Bulkhead Insulation
Release Rate (ng / g PCB-day)
1000000
100000
10000
1000
0
2
4
6
8
10
12
14
16
Time in Years
Predicted
Observed

Hexachlorobiphenyl in Bulkhead Insulation

ng/ g-PCB - d	C16
0.007	0
1.170	0
7.076	15830
14.083	16417
21.097	42170
42.226	17305
69.301	53159
83.139	46997
118.135	20906
167.104	50089
209.131	18376
251.192	19120
286.150	8972
328.092	13422
370.117	9568
398.079	18897
454.319	9396

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
4.24E+00	69.301	53159	1.09E+01
4.42E+00	83.139	46997	1.08E+01
4.77E+00	118.135	20906	9.95E+00
5.12E+00	167.104	50089	1.08E+01
5.34E+00	209.131	18376	9.82E+00
5.53E+00	251.192	19120	9.86E+00
5.66E+00	286.150	8972	9.10E+00
5.79E+00	328.092	13422	9.50E+00
5.91E+00	370.117	9568	9.17E+00
5.99E+00	398.079	18897	9.85E+00
6.12E+00	454.319	9396	9.15E+00

Maximum Release Rate at 69 days
53159 ng/gPCB-d

Release rate at 2 years
6762 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.8352
R Square	0.6976
Standard Error	0.3870
Observations	11

ANOVA

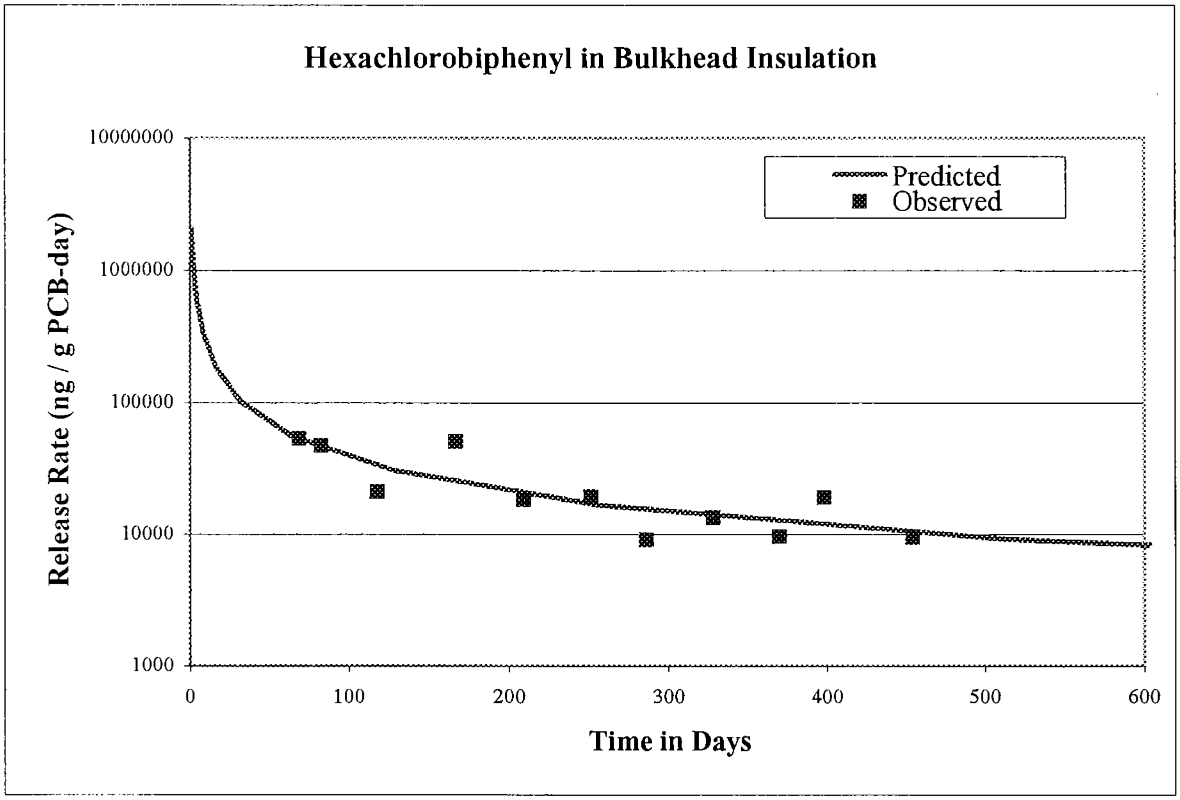
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	3.11E+00	3.11E+00	2.08E+01	1.37E-03
Residual	9	1.35E+00	1.50E-01		
Total	10	4.46E+00			

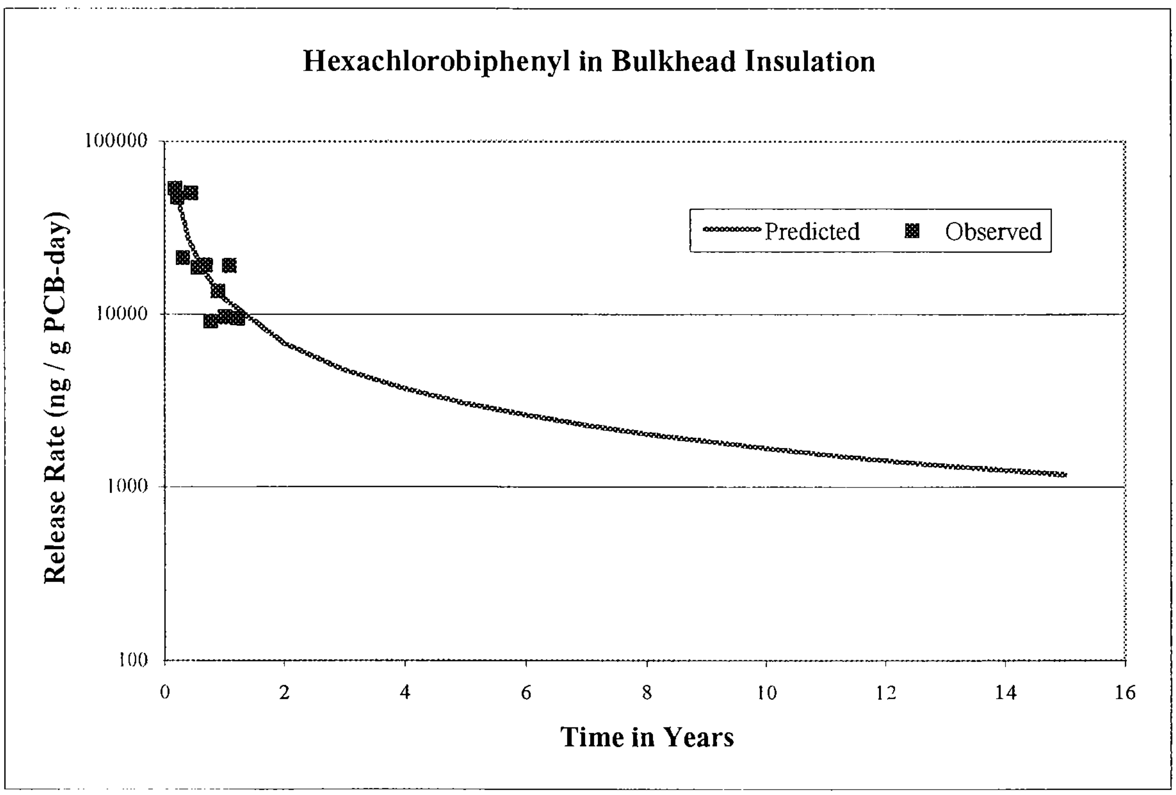
	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	1.45E+01	1.03E+00	1.42E+01	1.86E-07	1.22E+01	1.69E+01
ln(day)	-8.69E-01	1.91E-01	-4.56E+00	1.37E-03	-1.30E+00	-4.37E-01

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	1.09E+01	1.69E-02
2	1.07E+01	5.18E-02
3	1.04E+01	-4.53E-01
4	1.01E+01	7.22E-01
5	9.90E+00	-8.60E-02
6	9.75E+00	1.13E-01
7	9.63E+00	-5.31E-01
8	9.51E+00	-9.06E-03
9	9.41E+00	-2.43E-01
10	9.35E+00	5.01E-01

11	9.23E+00	-8.30E-02





Heptaachlorobiphenyl in Bulkhead Insulation

ng/ g-PCB - d	Cl7
0.007	0
1.170	34568
7.076	5919
14.083	3694
21.097	0
42.226	0
69.301	0
83.139	4406
118.135	0
167.104	3695
209.131	1838
251.192	0
286.150	0
328.092	0
370.117	0
398.079	0
454.319	0

ln(day)	day	ng/gPCB-d	ln(ng/g-PCB-d)
1.57E-01	1.170	34568	1.05E+01
1.96E+00	7.076	5919	8.69E+00
2.64E+00	14.083	3694	8.21E+00
4.42E+00	83.139	4406	8.39E+00
5.12E+00	167.104	3695	8.21E+00
5.34E+00	209.131	1838	7.52E+00

Maximum Release Rate at 1 day
34568 ng/gPCB-d

Release rate at 2 years
1303 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.8699
R Square	0.7568
Standard Error	0.5484
Observations	6

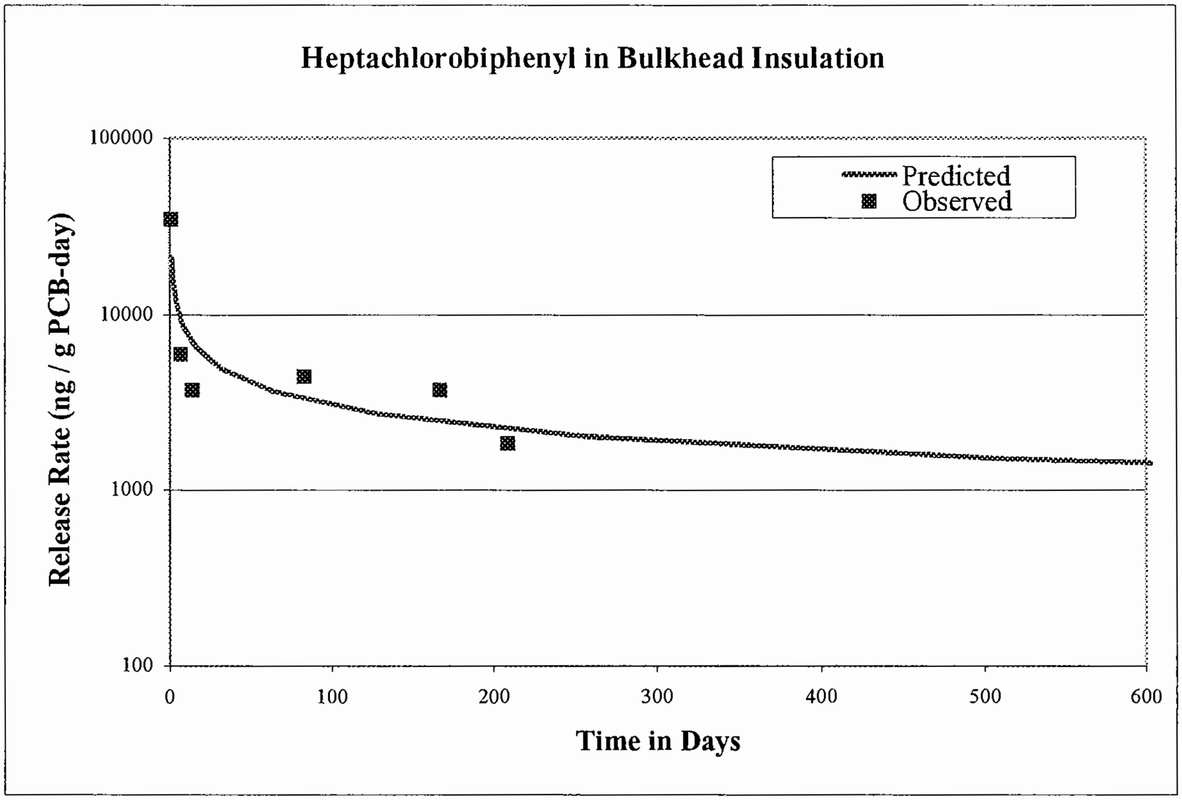
ANOVA

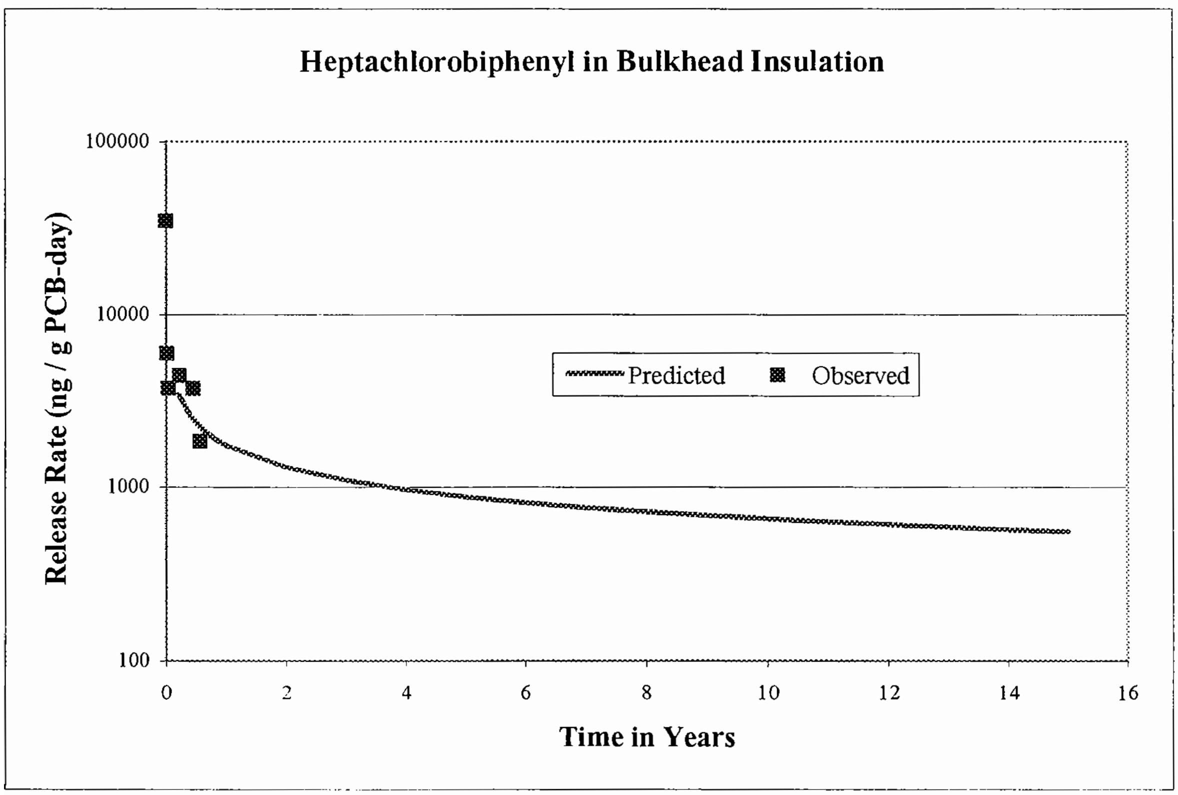
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	3.74E+00	3.74E+00	1.24E+01	2.43E-02
Residual	4	1.20E+00	3.01E-01		
Total	5	4.95E+00			

	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	9.97E+00	4.52E-01	2.20E+01	2.51E-05	8.71E+00	1.12E+01
ln(day)	-4.24E-01	1.20E-01	-3.53E+00	2.43E-02	-7.57E-01	-9.02E-02

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	9.90E+00	5.51E-01
2	9.14E+00	-4.51E-01
3	8.85E+00	-6.31E-01
4	8.09E+00	2.98E-01
5	7.80E+00	4.18E-01
6	7.70E+00	-1.86E-01


Heptachlorobiphenyl in Bulkhead Insulation
Release Rate (ng / g PCB-day)
100000
10000
1000
100
0
100
200
300
400
500
600
Time in Days
Predicted
Observed


Heptachlorobiphenyl in Bulkhead Insulation
Release Rate (ng / g PCB-day)
100000
10000
1000
100
0
2
4
6
8
10
12
14
16
Time in Years
Predicted
Observed

ELECTRICAL CABLE INSULATION

Electrical Cable

Leaching Time (days)	Homologue Leach Rates (ng PCB/g shipboard solid-day)									
	Cl1	Cl2	Cl3	Cl4	Cl5	Cl6	Cl7	Cl8	Cl9	Cl10
0.002777778	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
1.077083333	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
6.009027778	0.0E+00	3.4E-01	0.0E+00	5.9E-02	1.2E-01	0.0E+00	2.4E-02	0.0E+00	0.0E+00	0.0E+00
20.03541667	0.0E+00	0.0E+00	0.0E+00	6.1E-02	7.8E-02	6.6E-03	2.2E-02	0.0E+00	0.0E+00	0.0E+00
40.98888889	0.0E+00	9.9E-03	1.0E-03	6.5E-02	1.1E-01	2.6E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00
62.23541667	0.0E+00	0.0E+00	0.0E+00	5.1E-02	9.9E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
90.00972222	0.0E+00	2.2E-02	0.0E+00	4.2E-02	7.3E-02	2.6E-02	4.9E-03	0.0E+00	0.0E+00	0.0E+00
125.0284722	0.0E+00	0.0E+00	1.9E-03	4.0E-02	6.7E-02	4.0E-02	0.0E+00	0.0E+00	2.5E-03	1.4E-03
166.9979167	0.0E+00	0.0E+00	0.0E+00	3.6E-02	7.3E-02	2.3E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00
208.9680556	0.0E+00	0.0E+00	0.0E+00	3.3E-02	7.4E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
250.9819444	0.0E+00	0.0E+00	0.0E+00	3.2E-02	4.4E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
300.0243056	0.0E+00	0.0E+00	0.0E+00	2.5E-02	1.6E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
341.9638889	0.0E+00	0.0E+00	0.0E+00	2.7E-02	4.1E-02	9.9E-03	0.0E+00	0.0E+00	0.0E+00	0.0E+00
383.9930556	0.0E+00	0.0E+00	0.0E+00	4.3E-02	5.3E-02	1.7E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00
411.9548611	0.0E+00	0.0E+00	0.0E+00	5.8E-02	9.1E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
474.98125	0.0E+00	0.0E+00	0.0E+00	2.1E-02	2.3E-02	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00
Max	0.0E+00	3.4E-01	1.9E-03	6.5E-02	1.2E-01	4.0E-02	2.4E-02	0.0E+00	2.5E-03	1.4E-03
Min	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00

0.0012 g PCB / g electrical cable (leachate study concentration) - ratio of intact cable to cable insulation = 0.7226)

Leaching Time (days)	Homologue Leach Rates (ng PCB/g PCB-day)									
ng/ g-PCB - d	Cl1	Cl2	Cl3	Cl4	Cl5	Cl6	Cl7	Cl8	Cl9	Cl10
0.002777778	0	0	0	0	0	0	0	0	0	0
1.077083333	0	0	0	0	0	0	0	0	0	0
6.009027778	0	203	0	35.5	73	0	14.7	0	0	0
20.03541667	0	0	0	36.8	47.1	3.97	13.1	0	0	0
40.98888889	0	5.98	0.617	38.8	63.7	15.9	0	0	0	0
62.23541667	0	0	0	30.4	59.9	0	0	0	0	0
90.00972222	0	13.3	0	25.3	44.2	15.5	2.95	0	0	0
125.0284722	0	0	1.14	24.1	40.4	24.1	0	0	1.51	0.84
166.9979167	0	0	0	21.6	44.2	14.1	0	0	0	0
208.9680556	0	0	0	19.8	44.7	0	0	0	0	0
250.9819444	0	0	0	19.4	26.3	0	0	0	0	0
300.0243056	0	0	0	14.9	9.4	0	0	0	0	0
341.9638889	0	0	0	16.4	24.9	5.97	0	0	0	0
383.9930556	0	0	0	25.6	32.1	10.0	0	0	0	0
411.9548611	0	0	0	34.7	55.1	0	0	0	0	0
474.98125	0	0	0	12.7	14.1	0	0	0	0	0
Max	0	203	1.14	38.8	73.5	24.1	14.7	0	1.51	0.843
Min	0	0	0	0	0	0	0	0	0	0
Median	0	0	0	22.9	42.3	0	0	0	0	0
Simple Avergae	0	13.9	0	22.2	36.2	5.60	1.92	0	0	0
Detects	0	3	2	14	14	7	3	0	1	1
Non-detects	15	12	13	1	1	8	12	15	14	14
Intercept	---	7.11E+00	---	5.60E-01	5.93E+00	7.61E+00	4.00E+00	---	---	---
Slope	---	-1.16E+00	---	-2.62E-01	-4.62E-01	-9.45E-01	-6.10E-01	---	---	---
alpha	---	3.22E-01	---	3.30E-02	3.05E-02	1.20E-01	2.52E-01	---	---	---

Dichlorobiphenyl in Electrical Cable Insulation

ng/ g-PCB - d	Cl2
2.78E-03	0
1.08E+00	0
6.01E+00	203
2.00E+01	0
4.10E+01	6
6.22E+01	0
9.00E+01	13
1.25E+02	0
1.67E+02	0
2.09E+02	0
2.51E+02	0
3.00E+02	0
3.42E+02	0
3.84E+02	0
4.12E+02	0
4.75E+02	0

ln(d)	day	ng/gPCB-d	ln(ng/g-PCB-d)
1.79E+00	6.01E+00	203	5.31E+00
3.71E+00	4.10E+01	6	1.79E+00
4.50E+00	9.00E+01	13	2.59E+00

Maximum Release Rate at 6 days
203 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.8749
R Square	0.7655
Standard Error	1.2657
Observations	3

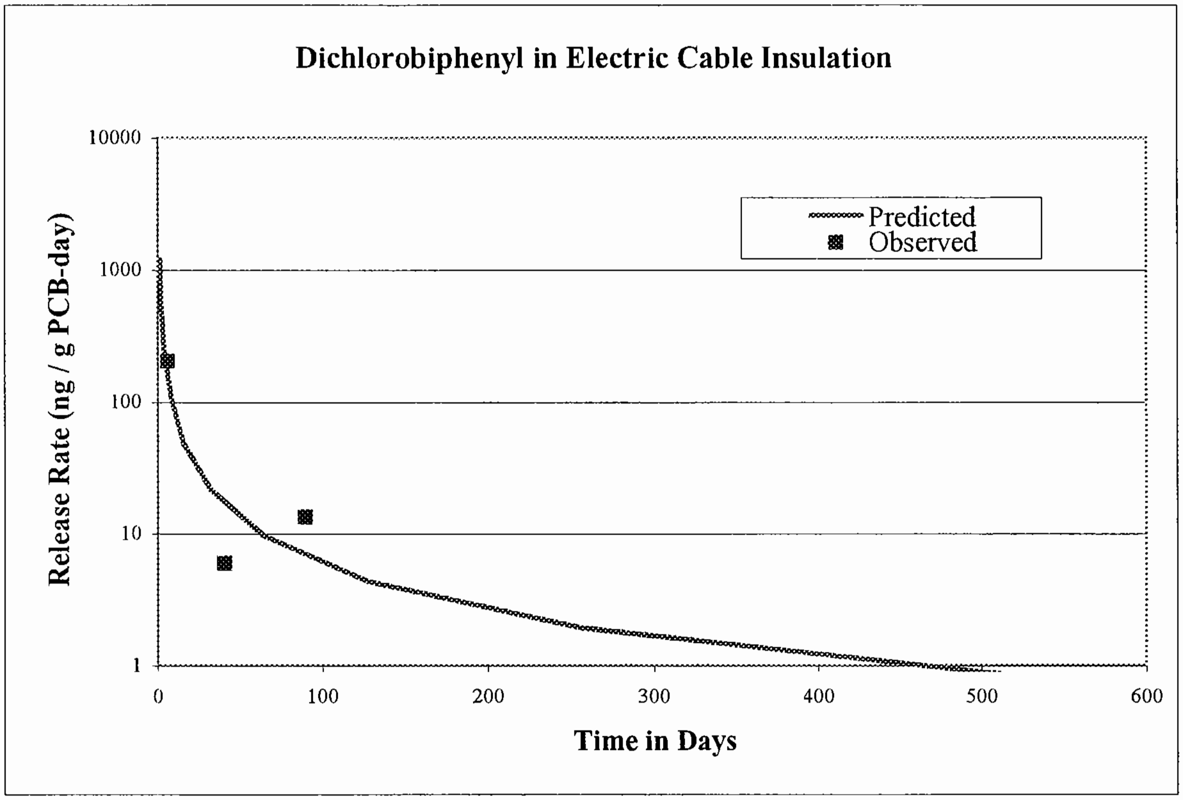
ANOVA

	df	*SS*	*MS*	*F*	*Significance F*	
Regression	1	5.23E+00	5.23E+00	3.26E+00	3.22E-01	***Not Significant***
Residual	1	1.60E+00	1.60E+00			
Total	2	6.83E+00				

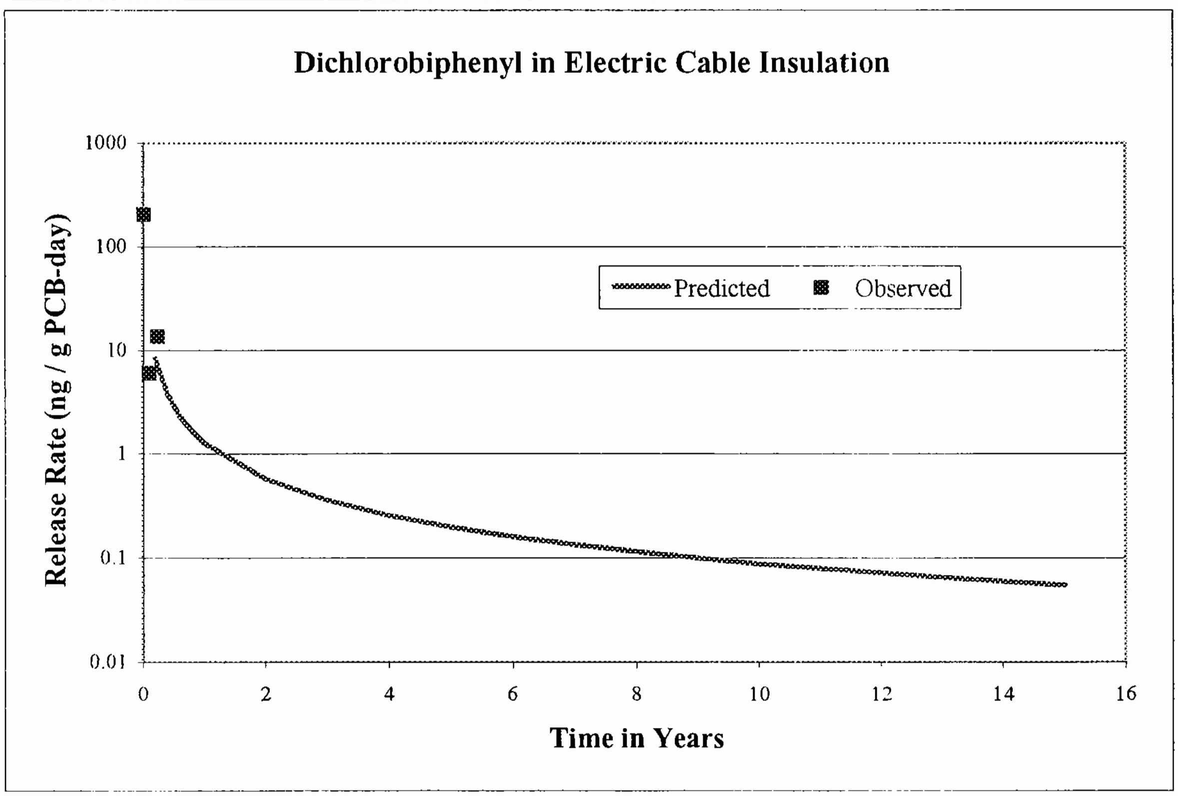
	Coefficients	*andard Erro*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	7.11E+00	2.27E+00	3.14E+00	1.96E-01	-2.17E+01	3.59E+01
ln(d)	-1.16E+00	6.43E-01	-1.81E+00	3.22E-01	-9.33E+00	7.01E+00

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	5.02E+00	2.92E-01
2	2.79E+00	-1.00E+00
3	1.88E+00	7.13E-01



Dichlorobiphenyl in Electric Cable Insulation
Release Rate (ng / g PCB-day)
10000
1000
100
10
1
Predicted
Observed
0
100
200
300
400
500
600
Time in Days



Dichlorobiphenyl in Electric Cable Insulation
Release Rate (ng / g PCB-day)
1000
100
10
1
0.1
0.01
Predicted
Observed
0
2
4
6
8
10
12
14
16
Time in Years

Pentachlorobiphenyl in Electrical Cable Insulation

ng/ g-PCB - d	Cl5
2.78E-03	0
1.08E+00	0
6.01E+00	73.5
2.00E+01	47.1
4.10E+01	63.7
6.22E+01	59.9
9.00E+01	44.2
1.25E+02	40.4
1.67E+02	44.2
2.09E+02	44.7
2.51E+02	26.3
3.00E+02	9.4
3.42E+02	24.9
3.84E+02	32.1
4.12E+02	55.1
4.75E+02	14.1

ln(d)	day	ng/gPCB-d	ln(ng/g-PCB-d)
3.71E+00	40.989	63.7	4.15E+00
4.13E+00	62.235	59.9	4.09E+00
4.50E+00	90.010	44.2	3.79E+00
4.83E+00	125.028	40.4	3.70E+00
5.12E+00	166.998	44.2	3.79E+00
5.34E+00	208.968	44.7	3.80E+00
5.53E+00	250.982	26.3	3.27E+00
5.70E+00	300.024	9.4	2.24E+00
5.83E+00	341.964	24.9	3.21E+00
5.95E+00	383.993	32.1	3.47E+00
6.02E+00	411.955	55.1	4.01E+00
6.16E+00	474.981	14.1	2.64E+00

Maximum Release Rate at 40 days
63.7 ng/gPCB-d

Release rate at 2 years
18.0 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.6229
R Square	0.3880
Standard Error	0.4823
Observations	12

ANOVA

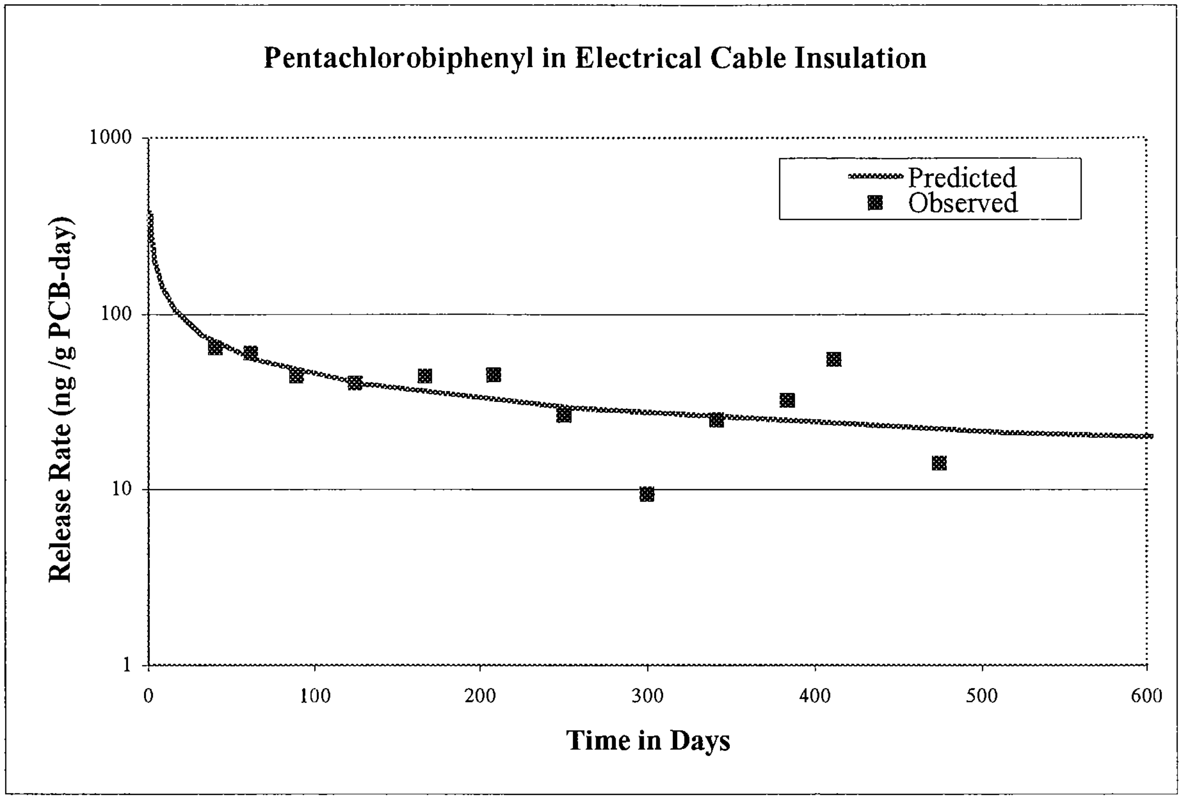
	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.47E+00	1.47E+00	6.34E+00	3.05E-02
Residual	10	2.33E+00	2.33E-01		
Total	11	3.80E+00			

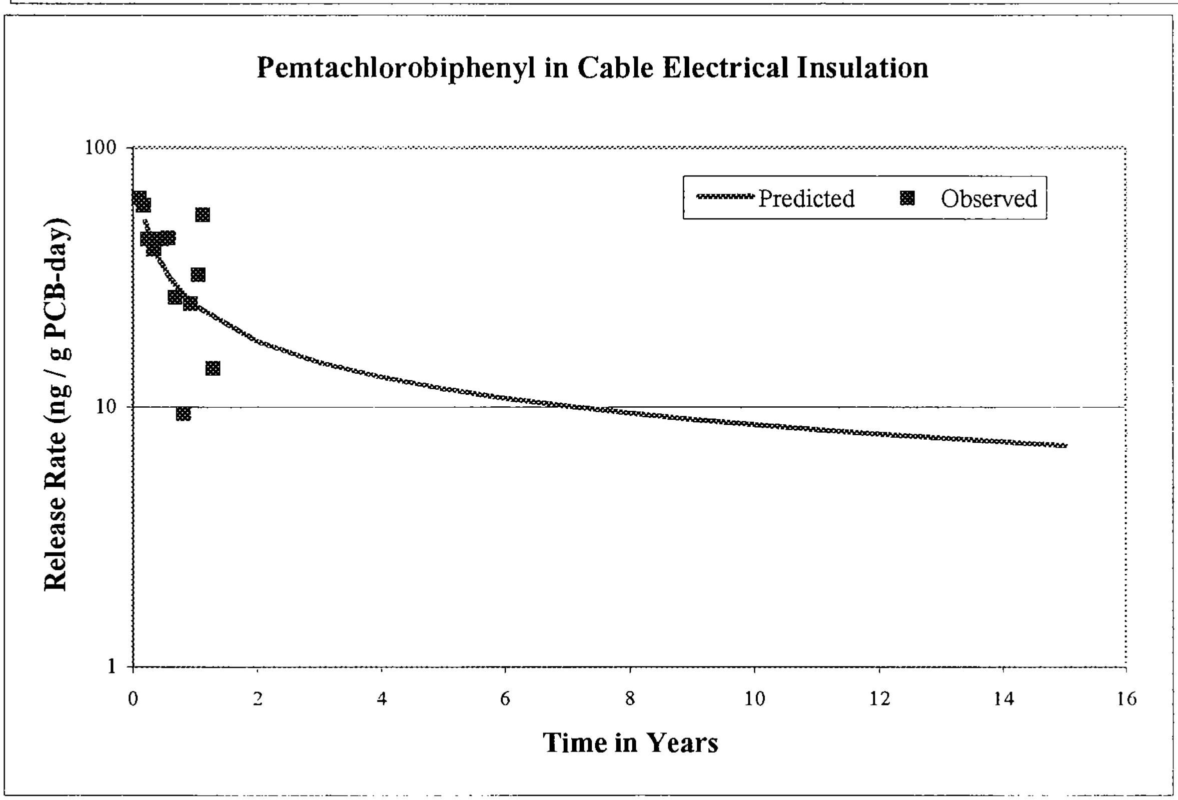
	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	5.93E+00	9.70E-01	6.11E+00	1.13E-04	3.77E+00	8.09E+00
ln(d)	-4.62E-01	1.83E-01	-2.52E+00	3.05E-02	-8.70E-01	-5.31E-02

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	4.22E+00	-6.20E-02
2	4.02E+00	6.88E-02
3	3.85E+00	-6.39E-02
4	3.70E+00	-4.23E-03
5	3.57E+00	2.21E-01
6	3.47E+00	3.36E-01
7	3.38E+00	-1.10E-01
8	3.30E+00	-1.06E+00
9	3.24E+00	-2.37E-02
10	3.18E+00	2.85E-01

11	3.15E+00	8.57E-01
12	3.09E+00	-4.43E-01





Hexachlorobiphenyl in Electrical Cable Insulation

ng/ g-PCB - d	Cl6
2.78E-03	0
1.08E+00	0
6.01E+00	0.0
2.00E+01	4.0
4.10E+01	15.9
6.22E+01	0.0
9.00E+01	15.5
1.25E+02	24.1
1.67E+02	14.1
2.09E+02	0.0
2.51E+02	0.0
3.00E+02	0.0
3.42E+02	6.0
3.84E+02	10.0
4.12E+02	0.0
4.75E+02	0.0

ln(d)	day	ng/gPCB-d	ln(ng/g-PCB-d)
4.83E+00	1.25E+02	24.1	3.18E+00
5.12E+00	1.67E+02	14.1	2.64E+00
5.83E+00	3.42E+02	6.0	1.79E+00
5.95E+00	3.84E+02	10.0	2.31E+00

Maximum Release Rate at 125 days
24.1 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.8798
R Square	0.7741
Standard Error	0.3411
Observations	4

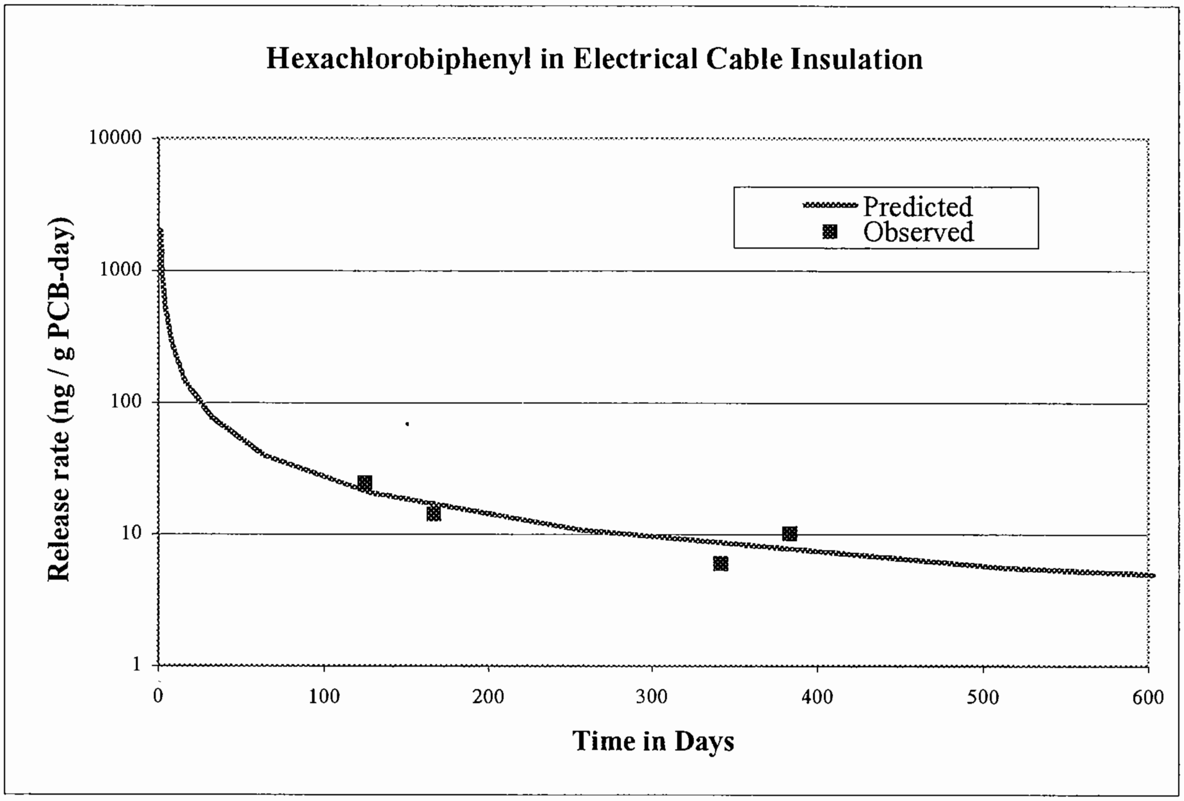
ANOVA

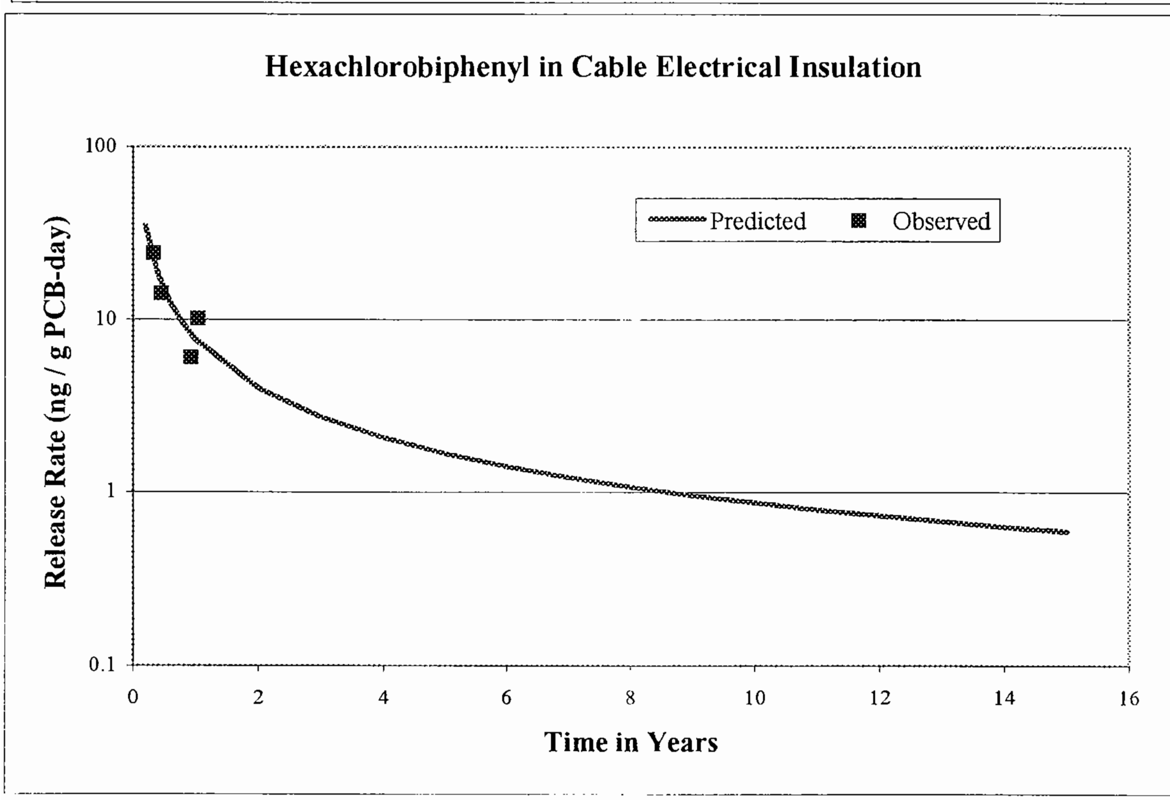
	df	*SS*	*MS*	*F*	*Significance F*	
Regression	1	7.98E-01	7.98E-01	6.85E+00	1.20E-01	***Not Significant***
Residual	2	2.33E-01	1.16E-01			
Total	3	1.03E+00				

	Coefficients	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	7.61E+00	1.97E+00	3.87E+00	6.08E-02	-8.55E-01	1.61E+01
ln(d)	-9.45E-01	3.61E-01	-2.62E+00	1.20E-01	-2.50E+00	6.08E-01

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	3.05E+00	1.31E-01
2	2.78E+00	-1.33E-01
3	2.10E+00	-3.14E-01
4	1.99E+00	3.15E-01


Hexachlorobiphenyl in Electrical Cable Insulation
Predicted
Observed
Release rate (ng / g PCB-day)
10000
1000
100
10
1
0
100
200
300
400
500
600
Time in Days


Hexachlorobiphenyl in Cable Electrical Insulation
Predicted
Observed
Release Rate (ng / g PCB-day)
100
10
1
0.1
0
2
4
6
8
10
12
14
16
Time in Years

Heptachlorobiphenyl in Electrical Cable Insulation

ng/ g-PCB - d	Cl7
2.78E-03	0
1.08E+00	0
6.01E+00	14.7
2.00E+01	13.1
4.10E+01	0
6.22E+01	0
9.00E+01	2.95
1.25E+02	0
1.67E+02	0
2.09E+02	0
2.51E+02	0
3.00E+02	0
3.42E+02	0
3.84E+02	0
4.12E+02	0
4.75E+02	0

ln(d)	day	ng/gPCB-d	ln(ng/g-PCB-d)
1.79E+00	6.01E+00	14.7	2.69E+00
3.00E+00	2.00E+01	13.1	2.57E+00
4.50E+00	9.00E+01	2.95	1.08E+00

Maximum Release Rate at 6 days
14.7 ng/gPCB-d

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.9227
R Square	0.8515
Standard Error	0.4882
Observations	3

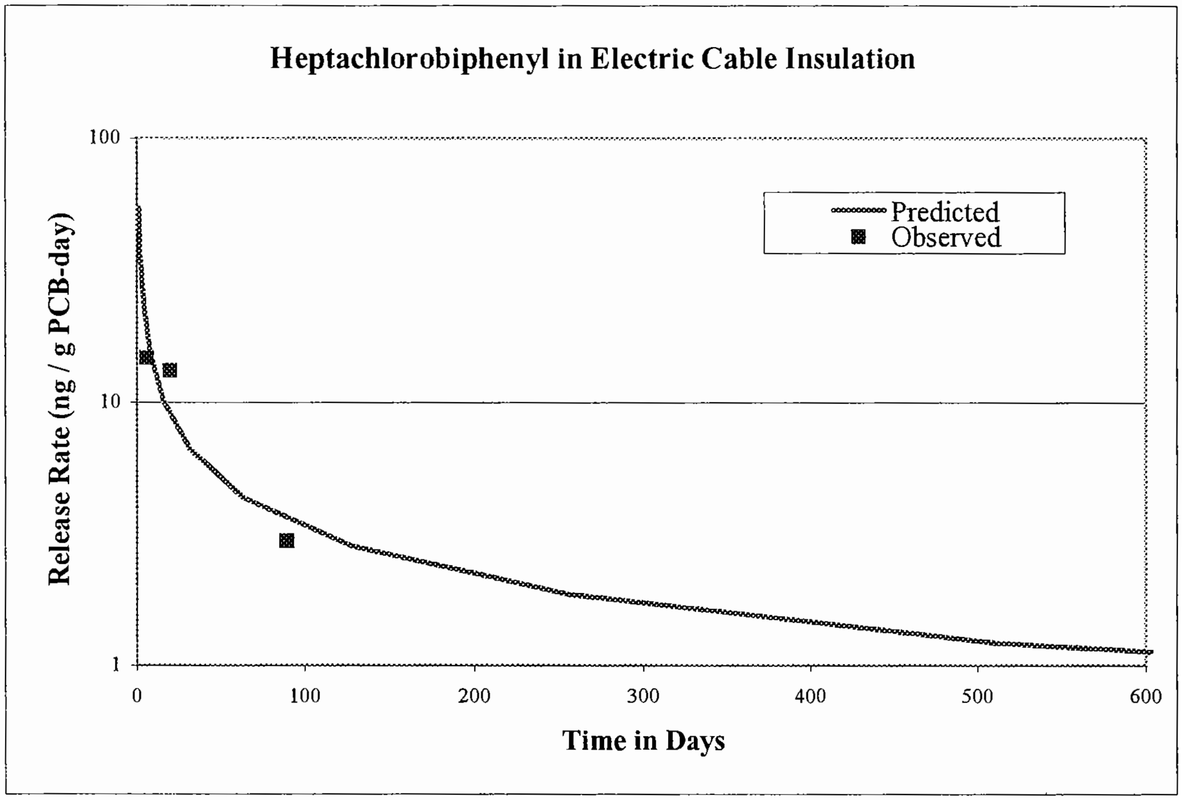
ANOVA

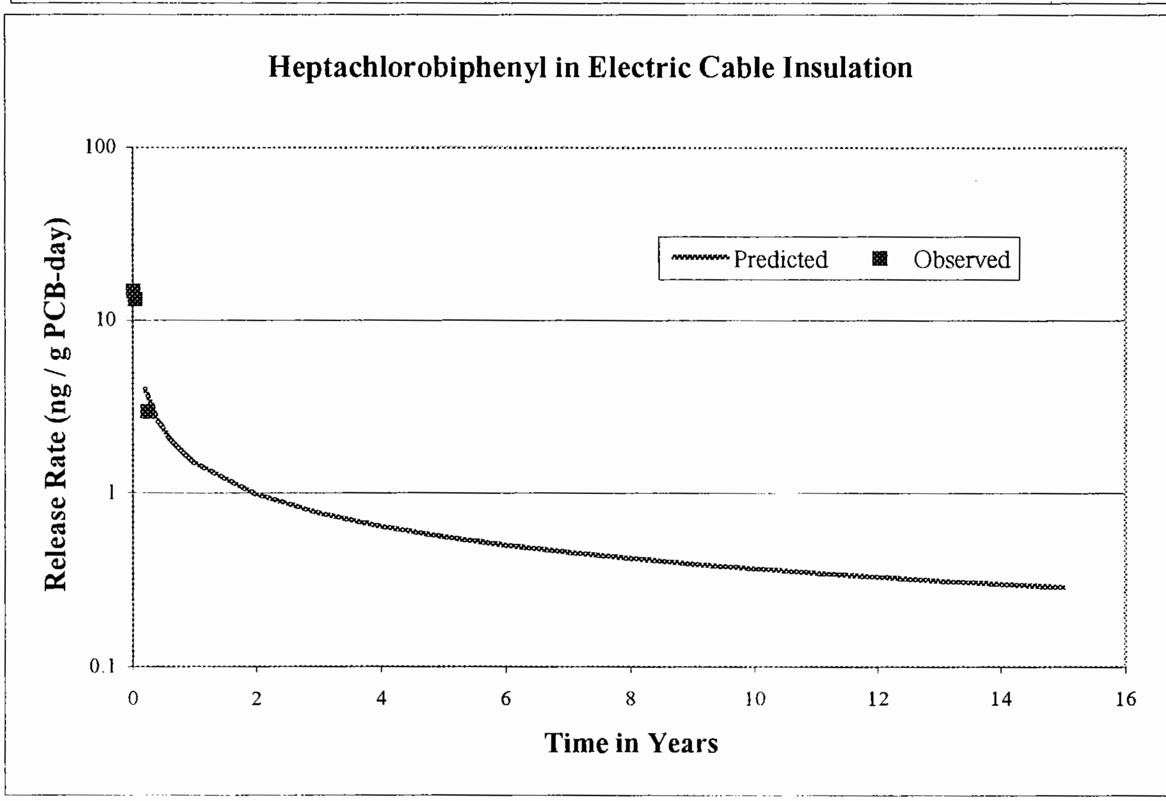
	df	*SS*	*MS*	*F*	*Significance F*	
Regression	1	1.37E+00	1.37E+00	5.73E+00	2.52E-01	***Not Significant***
Residual	1	2.38E-01	2.38E-01			
Total	2	1.60E+00				

	Coefficients	*andard Erro*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	4.00E+00	8.37E-01	4.78E+00	1.31E-01	-6.64E+00	1.46E+01
ln(d)	-6.10E-01	2.55E-01	-2.39E+00	2.52E-01	-3.84E+00	2.63E+00

RESIDUAL OUTPUT

Observation	*icted ln(ng/g-PC*	*Residuals*
1	2.91E+00	-2.21E-01
2	2.17E+00	3.98E-01
3	1.26E+00	-1.77E-01


Heptachlorobiphenyl in Electric Cable Insulation
100
10
1
Release Rate (ng / g PCB-day)
0
100
200
300
400
500
600
Time in Days
Predicted
Observed


Heptachlorobiphenyl in Electric Cable Insulation
100
10
1
0.1
Release Rate (ng / g PCB-day)
0
2
4
6
8
10
12
14
16
Time in Years
Predicted
Observed

MATERIAL FRACTIONS

PCB Concentrations in Cable Onboard the Ex-ORISKANY

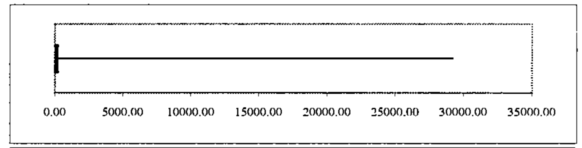
There is a sufficient number of values for statistical analysis - the data were found to be non-normal with high skewness, however, the Hall's transformed t bootstrap failed to normalize the dataset - use the Standard Bootstrap mean and UCLs as the EPCs

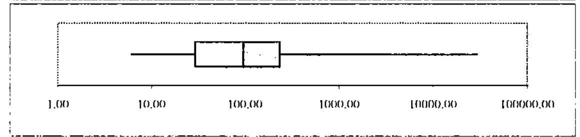
Units =	PPM	
Sample#	Value	Qualifier
95PS00034-001	110	
95PS00034-002	580	
95PS00034-003	10	
95PS00034-004	22	
95PS00034-005	9.5	
95PS00034-006	80	
95PS00034-007	67	
95PS00034-008	61	
95PS00034-009	38	
95PS00034-010	6.2	
95PS00034-011	400	
95PS00034-01	140	
95PS00034-01	290	
95PS00034-01	110	
95PS00034-01	2200	
95PS00034-01	5	U
95PS00034-01	56	
95PS00034-01	12000	
95PS00034-01	94	
95PS00034-02	85	
95PS00034-02	37	
95PS00034-02	24	
95PS00034-02	23	
95PS00034-02	12	
95PS00034-02	11000	
95PS00034-02	63	
95PS00034-02	100	
95PS00034-02	13	
95PS00034-02	45	
95PS00034-03	29000	
95PS00034-03	80	
95PS00034-03	150	
95PS00035-00	42	
95PS00035-00	290	
95PS00035-00	19000	
95PS00035-00	71	
95PS00035-00	30	
95PS00035-00	38	
95PS00035-00	85	
95PS00035-00	180	
95PS00035-00	95	
95PS00035-01	67	
95PS00035-01	59	
95PS00035-01	18	
95PS00035-01	65	
95PS00035-01	110	
95PS00032-01	580	
95PS00032-01	150	
95PS00032-01	140	
95PS00032-02	10000	
91NN00999-0	1	U
91NN00999-0	29	
91NN00999-0	78	
91NN00999-0	15	
91NN00999-0	33	
91NN00999-0	13	
91NN00999-0	23	
91NN00999-0	8	
91NN00999-0	70	

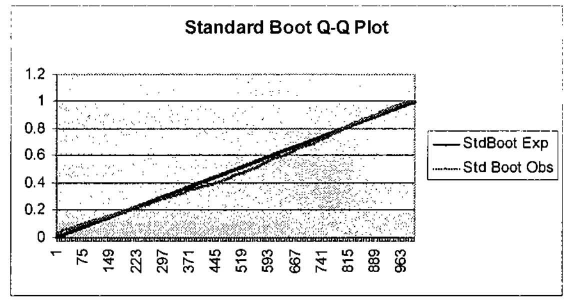
Low-End EPC	Bootstrap Mean	1494	
High-End EPC	Standard Bootstrap UCL	2559	

Raw Data Results			
Number of Samples	59		
Percent Detection	97% 57 of 59	Percent Detects J-coded	0%
Maximum Detection	2.90E+04	Minimum Detection	6.10E+00
Maximum Non-detection[1]	5.00E+00	Minimum Non-detection[1]	1.00E+00
Normal (Non-transformed) Results			
Normal Mean	1.49E+03	Mean Standard Error	6.49E+02
Standard Deviation	4.99E+03	Coefficient of Variance (%)	334%
Dataset Skewness	Fail 3.92E+00	Dataset Kurtosis	Fail 1.90E+01
Tested for Normality	D-Test	NormalityResult (a = 0.05)	Fail
Critical Value	-2.705 or 1.107	Calculated Value for dataset	-3.73E-01
90% UCL using t-statistic	2.34E+03	95% UCL using -t-statistic	2.58E+03
Natural Log-Transformed Results			
MVUE of the log-mean	6.20E+02	Standard error of the log-mean	2.50E+02
Standard Deviation	2.06E+00	Coefficient of Variance (%)	47%
Dataset Skewness	Fail 1.08E+00	Dataset Kurtosis	Pass 4.34E+00
Tested for Normality	D-Test	Normality Result (a = 0.05)	Fail
Critical Value	-2.705 or 1.107	Calculated Value for dataset	-5.70E+00
Anderson Darling (AD) A^2	2.19E+00	AD Probability	Fail 7.23E-02
90% UCL of the MVUE	1.42E+03	95% UCL of the MVUE	1.80E+03
EPA Concentration Term	1.80E+03	Chebychev 95% UCL	1.74E+03
Jackknife Results			
Jackknifed Mean	1.49E+03	Jackknifed Standard Error	6.49E+02
90% UCL of the mean	2.34E+03	95% UCL of the mean	2.58E+03
90% UCL of the MVUE[2]	1.03E+03	95% UCL of the MVUE[2]	1.18E+03

Bootstrap Results (Raw Data)							
Standard Bootstrap	Mean	1.49E+03	90% UCL	2.32E+03	95% UCL	2.56E+03	
Skewness	6.08E-01		Kurtosis	3.39E+00			
Quantile fit is good - Bootstrap Output is Normal or nearly so							
Pivitol (t) Bootstrap	90% UCL	2.86E+03	95% UCL	3.77E+03			
Skewness	-1.65E+01		Kurtosis	3.68E+02			
Quantile fit is poor do not use Bootstrap Results							
Hall's t Bootstrap	90% UCL	2.97E+03	95% UCL	3.85E+03			
Skewness	-2.73E+01		Kurtosis	7.90E+02			
Quantile fit is poor do not use Bootstrap Results							







Quantiles for the data set	
Minimum	6.10
Lower Quartile	23.0
Median	67.0
Upper Quartile	140
Maximum	29000

Percentiles of the bootstrap distribution	
5^{th} Percentile	525
25^{th} Percentile	1025
50^{th} Percentile	1421
75^{th} Percentile	1883
95^{th} Percentile	2685

1 = Equals 1/2 of the reporting limit
2 = Using the Jackknife

EPC=Environmental Exposure Concentration
MVUE=Minimum Variance Unbiased Estimator
UCL=Upper Confidence Interval

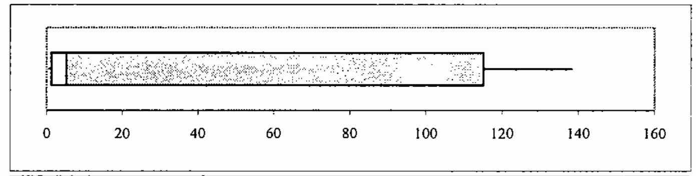
PCB Concentrations in Lubricants Onboard the Ex-ORISKANY

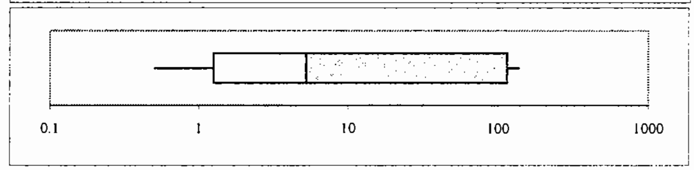
There is a sufficient number of values for statistical analysis - the data were found to be non-normally distributed and the number of samples is below 15 - use the Jackknife mean and UCL as the EPCs

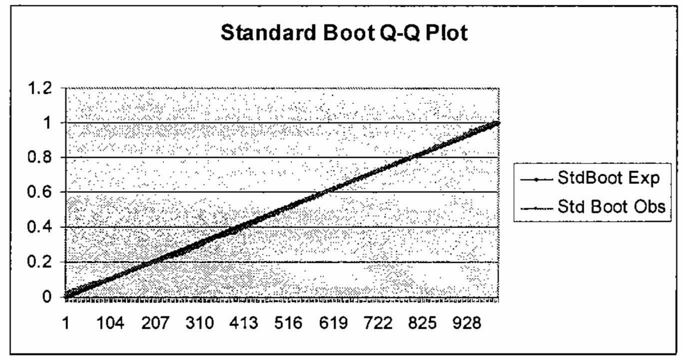
Units =	PPM	
Sample#	Value	Qualifier
91NN00999-001	0.5	U
95PS00029-001	150	
95PS00029-002	230	
95PS00029-003	0.5	U
95PS00029-004	0.5	U
95PS00029-005	4	
95PS00029-006	0.5	U
95PS00029-007	67	
95PS00029-008	100	
95PS00029-009	0.5	U
95PS00029-010	110	

Low-End EPC	Jackknife Mean		60.3		
High-End EPC	Jackknifed UCL		103		
Raw Data Results					
Number of Samples	11				
Percent Detection	55%	6 of 11	Percent Detects J-coded		0%
Maximum Detection	2.30E+02		Minimum Detection		4.00E+00
Maximum Non-detection[1]	5.00E-01		Minimum Non-detection[1]		5.00E-01
Normal (Non-transformed) Results					
Normal Mean	6.03E+01		Mean Standard Error		2.37E+01
Standard Deviation	7.87E+01		Coefficient of Variance (%)		131%
Dataset Skewness	Pass	8.46E-01	Dataset Kurtosis	Pass	2.31E+00
Tested for Normality	W-Test		NormalityResult (a = 0.05)		Fail
Critical Value	8.50E-01		Calculated Value for dataset		7.93E-01
90% UCL using t-statistic	9.29E+01		95% UCL using -t-statistic		1.03E+02
Natural Log-Transformed Results					
MVUE of the log-mean	1.25E+02		Standard error of the log-mean		1.01E+02
Standard Deviation	2.77E+00		Coefficient of Variance (%)		139%
Dataset Skewness	Pass	8.87E-02	Dataset Kurtosis	Fail	9.47E-01
Tested for Normality	W-Test		Normality Result (a = 0.05)		Fail
Critical Value	8.50E-01		Calculated Value for dataset		7.64E-01
Anderson Darling (AD) A^2	1.14E+00		AD Probability	Fail	2.90E-01
90% UCL of the MVUE	2.17E+04		95% UCL of the MVUE		1.43E+05
EPA Concentration Term	1.43E+05		Chebychev 95% UCL		5.78E+02
Jackknife Results					
Jackknifed Mean	6.03E+01		Jackknifed Standard Error		2.37E+01
90% UCL of the mean	9.29E+01		95% UCL of the mean		1.03E+02
90% UCL of the MVUE[2]	2.99E+02		95% UCL of the MVUE[2]		3.47E+02

Bootstrap Results (Raw Data)						
Standard Bootstrap	Mean	6.12E+01	90% UCL	8.99E+01	95% UCL	9.80E+01
Skewness	3.32E-01		Kurtosis	3.02E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Pivitol (t) Bootstrap	90% UCL	1.01E+02	95% UCL	1.17E+02		
Skewness	-1.30E+00		Kurtosis	8.49E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Hall's t Bootstrap	90% UCL	1.04E+02	95% UCL	1.20E+02		
Skewness	-1.22E+01		Kurtosis	2.11E+02		
Quantile fit is poor do not use Bootstrap Results						







Quantiles for the data set	
Minimum	0.5
Lower Quartile	0.76
Median	4
Upper Quartile	110
Maximum	23

Percentiles of the bootstrap distribution	
5th Percentile	26.8
25th Percentile	44.6
50th Percentile	60.6
75th Percentile	76.1
95th Percentile	99.9

1 = Equals 1/2 of the reporting limit
2 = Using the Jackknife

EPC=Environmental Exposure Concentration
MVUE=Minimum Variance Unbiased Estimator
UCL=Upper Confidence Interval

PCB Concentrations in Ventilation Gasket Material Onboard the Ex-ORISKANY

There is a sufficient number of values for statistical analysis - the data were found to be non-normal with high skewness, however, the Hall's transformed t bootstrap failed to normalize the dataset - use the Standard Bootstrap mean and UCLs as the EPCs

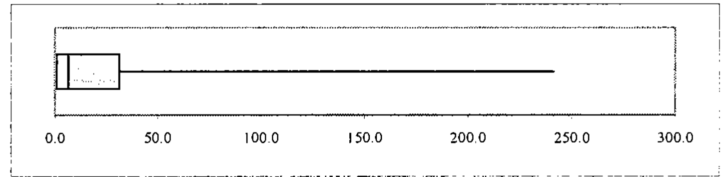
Units =	mg/kg	
Sample#	Value	Qualifier
91NN00999-045	0.5	U
91NN00999-047	0.5	U
91NN00999-049	7	
91NN00999-050	0.5	U
91NN00999-051	0.5	U
91NN00999-052	0.5	U
91NN00999-053	0.5	U
91NN00999-055	49	
91NN00999-056	0.5	U
91NN00999-058	22	
91NN00999-059	6	
91NN00999-060	5	
91NN00999-061	6	
91NN00999-062	210	
91NN00999-063	8	
91NN00999-064	11	
91NN00999-065	50	
91NN00999-068	13	
91NN00999-069	33	
91NN00999-070	0.5	U
91NN00999-071	0.5	U
91NN00999-072	5	
91NN00999-073	41	
91NN00999-074	0.5	U
91NN00999-075	78	
91NN00999-076	0.5	U
91NN00999-077	0.5	U
91NN00999-078	63	
91NN00999-079	0.5	U
91NN00999-081	35	
91NN00999-083	0.5	U
91NN00999-084	0.5	U
91NN00999-086	25	
91NN00999-087	15	

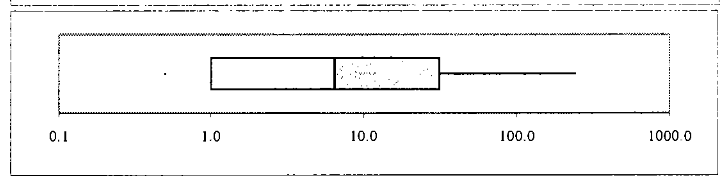
(Nondetect data presented as 1/2 the DL)

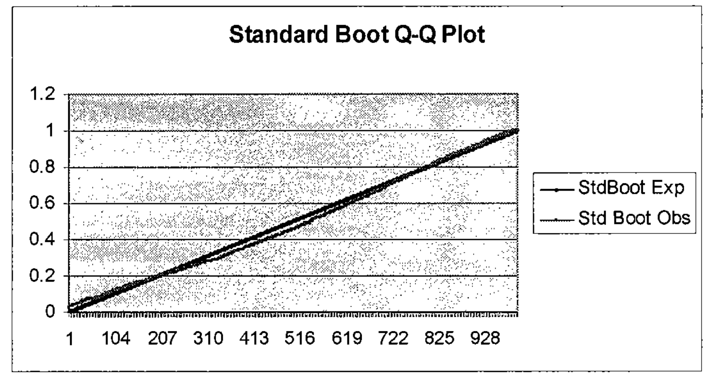
Low-End EPC	Bootstrap Mean	20.3	
High-End EPC	Standard Bootstrap UCL	31.5	

Raw Data Results			
Number of Samples	34		
Percent Detection	56% 19 of 34	Percent Detects J-coded	0%
Maximum Detection	2.10E+02	Minimum Detection	5.00E+00
Maximum Non-detection[1]	5.00E-01	Minimum Non-detection[1]	5.00E-01
Normal (Non-transformed) Results			
Normal Mean	2.03E+01	Mean Standard Error	6.74E+00
Standard Deviation	3.93E+01	Coefficient of Variance (%)	194%
Dataset Skewness	Fail 3.41E+00	Dataset Kurtosis	Fail 1.62E+01
Tested for Normality	W-Test	NormalityResult (a = 0.05)	Fail
Critical Value	9.33E-01	Calculated Value for dataset	5.53E-01
90% UCL using t-statistic	2.91E+01	95% UCL using -t-statistic	3.17E+01
Natural Log-Transformed Results			
MVUE of the log-mean	2.64E+01	Standard error of the log-mean	1.27E+01
Standard Deviation	2.03E+00	Coefficient of Variance (%)	147%
Dataset Skewness	Pass 2.07E-01	Dataset Kurtosis	Fail 1.46E+00
Tested for Normality	W-Test	Normality Result (a = 0.05)	Fail
Critical Value	9.33E-01	Calculated Value for dataset	8.25E-01
Anderson Darling (AD) A^2	2.36E+00	AD Probability	Fail 5.89E-02
90% UCL of the MVUE	8.36E+01	95% UCL of the MVUE	1.18E+02
EPA Concentration Term	1.18E+02	Chebychev 95% UCL	8.31E+01
Jackknife Results			
Jackknifed Mean	2.03E+01	Jackknifed Standard Error	6.74E+00
90% UCL of the mean	2.91E+01	95% UCL of the mean	3.17E+01
90% UCL of the MVUE[2]	4.28E+01	95% UCL of the MVUE[2]	4.73E+01

Bootstrap Results (Raw Data)						
Standard Bootstrap	Mean	2.03E+01	90% UCL	2.90E+01	95% UCL	3.15E+01
Skewness	7.76E-01		Kurtosis	3.66E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Pivitol (t) Bootstrap	90% UCL	3.72E+01	95% UCL	4.21E+01		
Skewness	-1.03E+00		Kurtosis	4.34E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Hall's t Bootstrap	90% UCL	3.88E+01	95% UCL	3.98E+01		
Skewness	-2.39E+00		Kurtosis	1.35E+01		
Quantile fit is poor do not use Bootstrap Results						







Quantiles for the data set	
Minimum	0.5
Lower Quartile	0.5
Median	5.5
Upper Quartile	25.0
Maximum	210

Percentiles of the bootstrap distribution	
5^{th} Percentile	10.7
25^{th} Percentile	15.6
50^{th} Percentile	20.3
75^{th} Percentile	24.7
95^{th} Percentile	32.1

1 = Equals 1/2 of the reporting limit
2 = Using the Jackknife

EPC=Environmental Exposure Concentration
MVUE=Minimum Variance Unbiased Estimator
UCL=Upper Confidence Interval

PCB Concentrations in Rubber Material Onboard the Ex-ORISKANY

There is a sufficient number of values for statistical analysis - the data were found to be non-normally distributed with high skewness - use the Standard Bootstrap mean and Hall's Adjusted Bootstrap UCLs as the EPCs

Units = mg/kg

Sample#	Value	Qualifier
95PS00032-001	32	
95PS00032-002	10	
95PS00032-003	24	
95PS00032-004	130	
95PS00032-005	6.5	
95PS00032-006	54	
95PS00032-007	29	
95PS00032-008	14	
95PS00032-009	2.5	U
95PS00032-010	19	
95PS00032-011	8.9	
95PS00035-015	12	
95PS00035-016	58	
95PS00035-017	2.5	U
95PS00035-018	110	
95PS00035-019	2.5	U
95PS00035-020	17	
95PS00035-021	46	
95PS00035-022	13	
95PS00035-023	2.5	U
95PS00035-024	28	
95PS00035-025	12	
95PS00035-026	110	
95PS00035-027	92	
95PS00035-028	39	
95PS00035-029	120	
95PS00035-030	33	
95PS00035-031	49	
95PS00035-032	42	
91NN00999-044	2.5	U

(Nondetect data presented as 1/2 the DL)

Low-End EPC	Bootstrap Mean	37.2
High-End EPC	Hall Adjusted Bootstrap	52.9

Raw Data Results

Number of Samples	30		
Percent Detection	83% 25 of 30	Percent Detects J-coded	0%
Maximum Detection	1.30E+02	Minimum Detection	6.50E+00
Maximum Non-detection[1]	2.50E+00	Minimum Non-detection[1]	2.50E+00

Normal (Non-transformed) Results

Normal Mean	3.74E+01	Mean Standard Error	6.95E+00
Standard Deviation	3.81E+01	Coefficient of Variance (%)	102%
Dataset Skewness	Fail 1.17E+00	Dataset Kurtosis	Pass 3.12E+00
Tested for Normality	W-Test	NormalityResult (a = 0.05)	Fail
Critical Value	9.27E-01	Calculated Value for dataset	8.12E-01
90% UCL using t-statistic	4.65E+01	95% UCL using -t-statistic	4.92E+01

Natural Log-Transformed Results

MVUE of the log-mean	4.25E+01	Standard error of the log-mean	1.17E+01
Standard Deviation	1.25E+00	Coefficient of Variance (%)	41%
Dataset Skewness	Pass -3.46E-01	Dataset Kurtosis	Pass 2.02E+00
Tested for Normality	W-Test	Normality Result (a = 0.05)	Fail
Critical Value	9.27E-01	Calculated Value for dataset	9.25E-01
Anderson Darling (AD) A^2	5.53E-01	AD Probability	Pass 6.93E-01
90% UCL of the MVUE	7.12E+01	95% UCL of the MVUE	8.38E+01
EPA Concentration Term	8.38E+01	Chebychev 95% UCL	9.48E+01

Jackknife Results

Jackknifed Mean	3.74E+01	Jackknifed Standard Error	6.95E+00
90% UCL of the mean	4.65E+01	95% UCL of the mean	4.92E+01
90% UCL of the MVUE[2]	5.55E+01	95% UCL of the MVUE[2]	5.92E+01

Bootstrap Results (Raw Data)

Standard Bootstrap	Mean	3.72E+01	90% UCL	4.63E+01	95% UCL	4.88E+01
Skewness	2.38E-01		Kurtosis	3.04E+00		

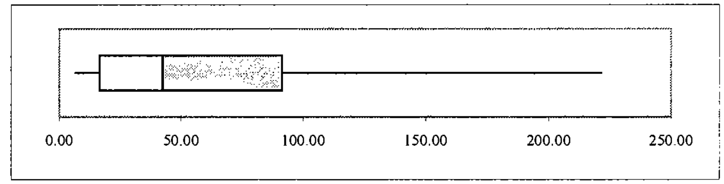
Quantile fit is good - Bootstrap Output is Normal or nearly so

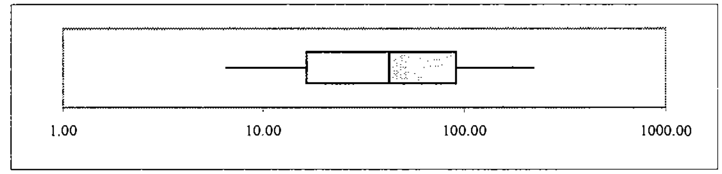
Pivitol (t) Bootstrap	90% UCL	4.81E+01	95% UCL	5.22E+01
Skewness	-9.47E-01	Kurtosis	6.05E+00	

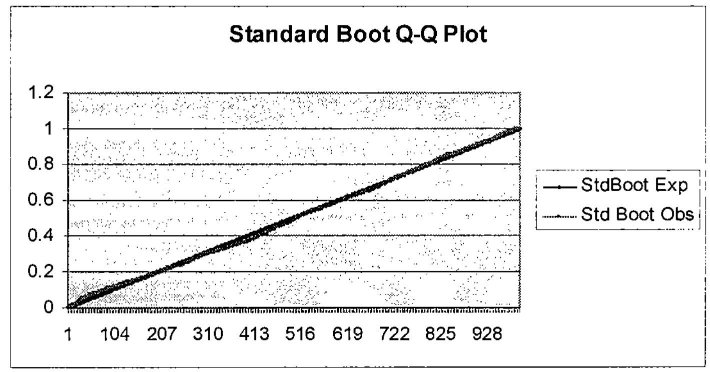
Quantile fit is good - Bootstrap Output is Normal or nearly so

Hall's t Bootstrap	90% UCL	4.75E+01	95% UCL	5.29E+01
Skewness	-2.02E+00	Kurtosis	1.15E+01	

Quantile fit is good - Bootstrap Output is Normal or nearly so







Quantiles for the data set	
Minimum	6.50
Lower Quartile	10.0
Median	26.0
Upper Quartile	49.0
Maximum	130

Percentiles of the bootstrap distribution	
5th Percentile	26.7
25th Percentile	32.1
50th Percentile	36.9
75th Percentile	41.9
95th Percentile	49.1

1 = Equals 1/2 of the reporting limit
2 = Using the Jackknife

EPC=Environmental Exposure Concentration
MVUE=Minimum Variance Unbiased Estimator
UCL=Upper Confidence Interval

PCB Concentrations in Paint Material Onboard the Ex-ORISKANY

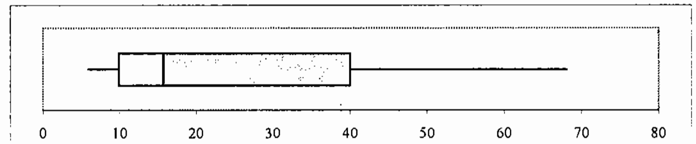
There is a sufficient number of values for statistical analysis - the data were found to be non-normally distributed and the number of samples is below 15 - use the Jackknife mean and UCL as the EPCs

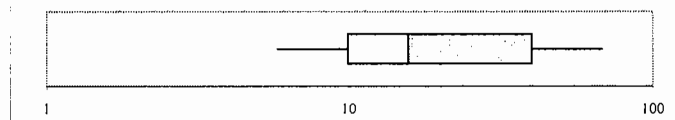
Units =	mg/kg	
Sample#	Value	Qualifier
Analab 7	24.4	
Analab 8	15.2	
95PS0032-012	5	U
95PS0032-013	5	U
95PS0032-014	5	U
95PS0032-015	28	
95PS0032-016	5.8	

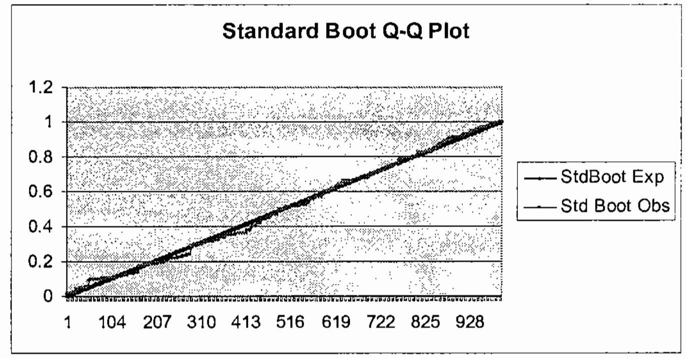
(Nondetect data presented as 1/2 the DL)

Low-End EPC	Jackknife Mean		12.6		
High-End EPC	Jackknifed UCL		20.0		
Raw Data Results					
Number of Samples	7				
Percent Detection	57%	4 of 7	Percent Detects J-coded	0%	
Maximum Detection	2.80E+01		Minimum Detection	5.80E+00	
Maximum Non-detection[1]	5.00E+00		Minimum Non-detection[1]	5.00E+00	
Normal (Non-transformed) Results					
Normal Mean	1.26E+01		Mean Standard Error	3.79E+00	
Standard Deviation	1.00E+01		Coefficient of Variance (%)	79%	
Dataset Skewness	Pass	5.15E-01	Dataset Kurtosis	Fail	1.24E+00
Tested for Normality	W-Test		NormalityResult (a = 0.05)	Fail	
Critical Value	8.03E-01		Calculated Value for dataset	7.77E-01	
90% UCL using t-statistic	1.81E+01		95% UCL using -t-statistic	2.00E+01	
Natural Log-Transformed Results					
MVUE of the log-mean	1.25E+01		Standard error of the log-mean	3.75E+00	
Standard Deviation	7.91E-01		Coefficient of Variance (%)	35%	
Dataset Skewness	Pass	3.38E-01	Dataset Kurtosis	Fail	9.91E-01
Tested for Normality	W-Test		Normality Result (a = 0.05)	Fail	
Critical Value	8.03E-01		Calculated Value for dataset	7.78E-01	
Anderson Darling (AD) A^2	7.22E-01		AD Probability	Pass	5.39E-01
90% UCL of the MVUE	2.59E+01		95% UCL of the MVUE	3.61E+01	
EPA Concentration Term	3.61E+01		Chebychev 95% UCL	2.92E+01	
Jackknife Results					
Jackknifed Mean	1.26E+01		Jackknifed Standard Error	3.79E+00	
90% UCL of the mean	1.81E+01		95% UCL of the mean	2.00E+01	
90% UCL of the MVUE[2]	1.84E+01		95% UCL of the MVUE[2]	2.05E+01	

Bootstrap Results (Raw Data)						
Standard Bootstrap	Mean	1.25E+01	90% UCL	1.71E+01	95% UCL	1.84E+01
Skewness	2.61E-01		Kurtosis	2.67E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Pivitol (t) Bootstrap	90% UCL	1.97E+01	95% UCL	2.95E+01		
Skewness	-6.61E+00		Kurtosis	4.71E+01		
Quantile fit is poor do not use Bootstrap Results						
Hall's t Bootstrap	90% UCL	1.97E+01	95% UCL	2.95E+01		
Skewness	-1.47E+01		Kurtosis	2.26E+02		
Quantile fit is poor do not use Bootstrap Results						







Quantiles for the data set	
Minimum	5.8
Lower Quartile	4.12
Median	5.8
Upper Quartile	24.4
Maximum	28

Percentiles of the bootstrap distribution	
5^{th} Percentile	6.80
25^{th} Percentile	9.74
50^{th} Percentile	12.5
75^{th} Percentile	14.9
95^{th} Percentile	18.7

1 = Equals 1/2 of the reporting limit
2 = Using the Jackknife

EPC=Environmental Exposure Concentration
MVUE=Minimum Variance Unbiased Estimator
UCL=Upper Confidence Interval

PCB Concentrations in Bulkhead Insulation Material Onboard the Ex-ORISKANY

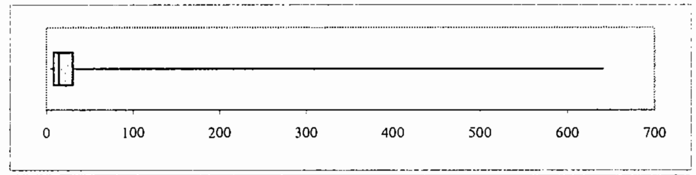
There is a sufficient number of values for statistical analysis - the data were found to be non-normal, however, the bootstrap methods failed to normalize the dataset - use the Jackknife mean and UCL as the EPCs

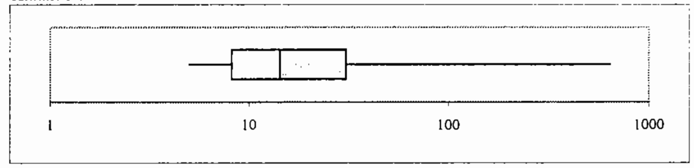
Units =	mg/kg	
Sample#	Value	Qualifier
95PS00019-002	6100	
95PS00019-023	320	
95PS00019-021	130	
95PS00019-003	60	
95PS00019-001	53	
95PS00019-004	45	
95PS00019-022	39	
95PS00019-014	18	
95PS00019-024	15	
95PS00019-011	11	
95PS00019-027	11	
95PS00019-015	7.4	
95PS00019-018	7.3	
95PS00019-025	6.9	
95PS00019-020	6.6	
95PS00019-017	6.4	
95PS00019-006	5.9	
95PS00019-019	5.5	
95PS00019-005	2.5	U
95PS00019-007	2.5	U
95PS00019-008	2.5	U
95PS00019-009	2.5	U
95PS00019-010	2.5	U
95PS00019-012	2.5	U
95PS00019-013	2.5	U
95PS00019-016	2.5	U
95PS00019-026	2.5	U
95PS00019-028	2.5	U
95PS00019-029	2.5	U
95PS00019-030	2.5	U
95PS00019-031	2.5	U
95PS00019-032	2.5	U

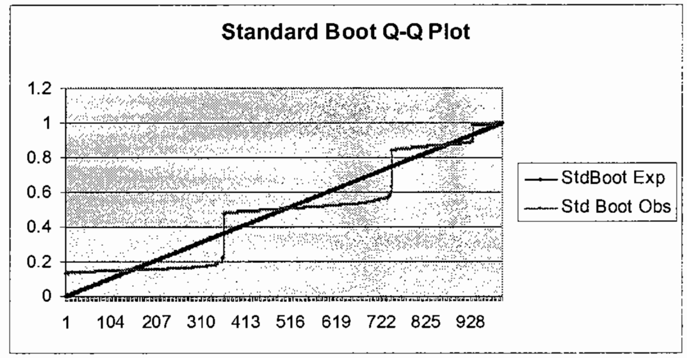
(Nondetect data presented as 1/2 the DL)

Low-End EPC	Jackknife Mean	215	
High-End EPC	Jackknifed UCL	537	

Raw Data Results					
Number of Samples	32				
Percent Detection	56%	18 of 32	Percent Detects J-coded		0%
Maximum Detection		6.10E+03	Minimum Detection		5.50E+00
Maximum Non-detection[1]		2.50E+00	Minimum Non-detection[1]		2.50E+00
Normal (Non-transformed) Results					
Normal Mean		2.15E+02	Mean Standard Error		1.90E+02
Standard Deviation		1.08E+03	Coefficient of Variance (%)		500%
Dataset Skewness	Fail	5.11E+00	Dataset Kurtosis	Fail	2.80E+01
Tested for Normality		W-Test	NormalityResult (a = 0.05)		Fail
Critical Value		9.30E-01	Calculated Value for dataset		2.06E-01
90% UCL using t-statistic		4.64E+02	95% UCL using -t-statistic		5.37E+02
Natural Log-Transformed Results					
MVUE of the log-mean		4.04E+01	Standard error of the log-mean		1.69E+01
Standard Deviation		1.78E+00	Coefficient of Variance (%)		80%
Dataset Skewness	Fail	1.79E+00	Dataset Kurtosis	Fail	6.37E+00
Tested for Normality		W-Test	Normality Result (a = 0.05)		Fail
Critical Value		9.30E-01	Calculated Value for dataset		7.57E-01
Anderson Darling (AD) A^2		2.47E+00	AD Probability	Fail	5.16E-02
90% UCL of the MVUE		1.03E+02	95% UCL of the MVUE		1.37E+02
EPA Concentration Term		1.37E+02	Chebychev 95% UCL		1.16E+02
Jackknife Results					
Jackknifed Mean		2.15E+02	Jackknifed Standard Error		1.90E+02
90% UCL of the mean		4.64E+02	95% UCL of the mean		5.37E+02
90% UCL of the MVUE[2]		6.73E+01	95% UCL of the MVUE[2]		7.79E+01
Bootstrap Results (Raw Data)					
Standard Bootstrap	Mean	2.09E+02	90% UCL	4.40E+02	95% UCL 5.06E+02
Skewness	8.81E-01		Kurtosis	3.59E+00	
Quantile fit is poor do not use Bootstrap Results					
Pivitol (t) Bootstrap	90% UCL	7.77E+03	95% UCL	1.15E+04	
Skewness	-2.70E+00		Kurtosis	1.18E+01	
Quantile fit is poor do not use Bootstrap Results					
Hall's t Bootstrap	90% UCL	6.91E+03	95% UCL	9.00E+03	
Skewness	-1.90E+01		Kurtosis	4.60E+02	
Quantile fit is poor do not use Bootstrap Results					







Quantiles for the data set	
Minimum	5
Lower Quartile	3.18
Median	6.15
Upper Quartile	16.5
Maximum	610

Percentiles of the bootstrap distribution	
5^{th} Percentile	13.2
25^{th} Percentile	28.7
50^{th} Percentile	210
75^{th} Percentile	387
95^{th} Percentile	590

1 = Equals 1/2 of the reporting limit
2 = Using the Jackknife

EPC=Environmental Exposure Concentration
MVUE=Minimum Variance Unbiased Estimator
UCL=Upper Confidence Interval

APPENDIX B

CALCULATION OF HOMOLOG-SPECIFIC K_{OW}s

OCTANOL TO WATER PARTITIONING COEFFICIENTS ($LOG_{10}K_{OW}$) FOR PCB CONGENERS AS OBTAINED FROM EISLER AND BELISLE (1996)

Monochlorobiphenyls		Dichlorobiphenyls		Trichlorobiphenyls		Tetrachlorobiphenyls		Pentachlorobiphenyls		Hexachlorobiphenyls		Heptachlorobiphenyls		Octachlorobiphenyls		Nonachlorobiphenyls		Decachlorobiphenyls	
1	4.601	4	5.023	16	5.311	40	5.561	82	6.142	128	6.961	170	7.277	194	8.683	206	9.143	209	9.603
2	4.421	5	NA	17	5.761	41	6.111	83	6.267	129	7.321	171	6.704	195	7.567	207	7.747		
3	4.401	6	5.021	18	5.551	42	5.767	84	6.041	130	7.391	172	7.337	196	7.657	208	8.164		
		7	5.15	19	5.481	43	5.757	85	6.611	131	6.587	173	7.027	197	7.307				
		8	5.301	20	5.577	44	5.811	86	6.204	132	6.587	174	7.117	198	7.627				
		9	5.18	21	5.17	45	5.537	87	6.371	133	6.867	175	7.177	199	7.207				
		10	5.311	22	5.421	46	5.537	88	7.516	134	7.304	176	6.767	200	7.277				
		11	5.343	23	5.577	47	6.291	89	6.077	135	7.151	177	7.087	201	7.627				
		12	5.295	24	5.671	48	5.787	90	6.367	136	6.511	178	7.147	202	8.423				
		13	NA	25	5.677	49	6.221	91	6.137	137	7.711	179	6.737	203	7.657				
		14	5.404	26	5.667	50	5.637	92	6.357	138	7.441	180	7.367	204	7.307				
		15	5.335	27	5.447	51	5.637	93	6.047	139	6.677	181	7.117	205	8.007				
				28	5.691	52	6.091	94	6.137	140	6.677	182	7.207						
				29	5.743	53	5.627	95	6.137	141	7.592	183	7.207						
				30	5.504	54	5.904	96	5.717	142	6.517	184	6.857						
				31	5.677	55	6.117	97	6.671	143	6.607	185	7.933						
				32	5.751	56	6.117	98	6.137	144	6.677	186	6.697						
				33	5.572	57	6.177	99	7.211	145	6.257	187	7.177						
				34	5.667	58	6.177	100	6.237	146	6.897	188	6.827						
				35	5.827	59	5.957	101	7.071	147	6.647	189	7.717						
				36	4.151	60	5.452	102	6.167	148	6.737	190	7.467						
				37	4.941	61	5.943	103	6.227	149	7.281	191	7.557						
				38	5.767	62	5.897	104	5.817	150	6.327	192	7.527						
				39	5.897	63	6.177	105	6.657	151	6.647	193	7.527						
						64	5.957	106	6.647	152	6.227								
						65	5.867	107	6.717	153	7.751								
						66	5.452	108	6.717	154	6.767								
						67	6.207	109	6.487	155	7.123								
						68	6.267	110	6.532	156	7.187								
						69	6.047	111	6.767	157	7.187								
						70	6.231	112	6.457	158	7.027								
						71	5.987	113	6.547	159	7.247								
						72	6.267	114	6.657	160	6.937								
						73	6.047	115	6.497	161	7.087								
						74	6.671	116	6.304	162	7.247								
						75	6.057	117	6.467	163	6.997								
						76	6.137	118	7.121	164	7.027								
						77	6.523	119	6.587	165	7.057								
						78	6.357	120	6.797	166	6.937								
						79	6.427	121	6.647	167	7.277								
						80	6.583	122	6.647	168	7.117								
						81	6.367	123	6.747	169	7.427								
								124	6.737										
								125	6.517										
								126	6.897										
								127	6.957										

NA = not available

STATISTICAL ANALYSIS OF OCTANOL-WATER PARTITIONING COEFFICIENTS OBTAINED FROM EISLER AND BELISLE (1996)

Dichlorobiphenyls

The data are best described as normally distributed and there were a sufficient number of detected values to perform a statistical analysis.

Congener	Value	$Log_{10}Kow$
4	105439	5.023
6	104954	5.021
7	141254	5.150
8	199986	5.301
9	151356	5.180
10	204644	5.311
11	220293	5.343
12	197242	5.295
14	253513	5.404
15	216272	5.335

No values were presented for congeners 5 and 13

Recommended Mean	Normal Mean	179495	Log_{10}	5.254
Recommended UCL	UCL based on t-statistic	208900	Log_{10}	5.320

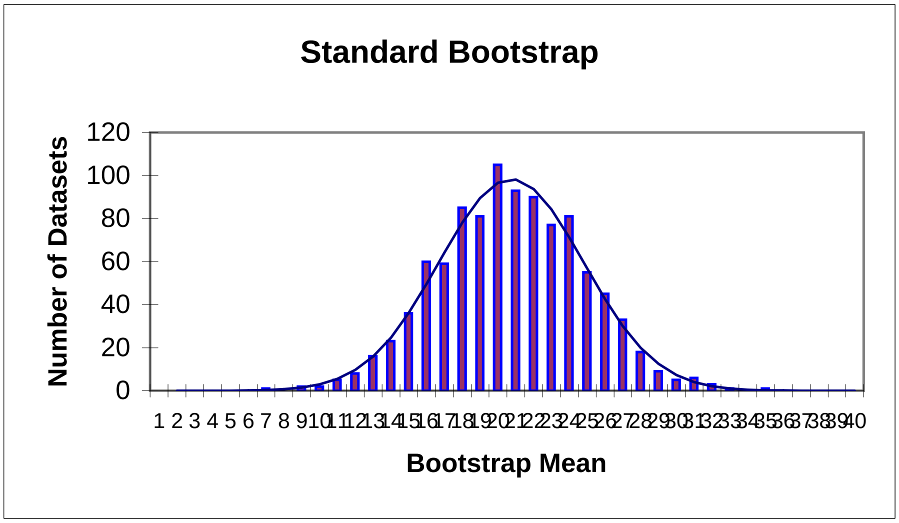
Raw Data Results					
Number of Values		10			
Maximum Value		2.54E+05	Minimum Value		1.05E+05
Normal (Non-transformed) Results					
Normal Mean		1.79E+05	Mean Standard Error		1.60E+04
Standard Deviation		5.07E+04	Coefficient of Variance (%)		28%
Dataset Skewness	Pass	-2.65E-01	Dataset Kurtosis	Fail	1.50E+00
Tested for Normality		W-Test	Normality Result (a = 0.05)		Pass
Critical Value		8.42E-01	Calculated Value for dataset		9.17E-01
90% UCL using t-statistic		2.02E+05	95% UCL using -t-statistic		2.09E+05
Natural Log-Transformed Results					
MVUE of the log-mean		1.80E+05	Standard error of the log-me		1.79E+04
Standard Deviation		3.12E-01	Coefficient of Variance (%)		3%
Dataset Skewness	Pass	-5.13E-01	Dataset Kurtosis	Fail	1.60E+00
Tested for Normality		W-Test	Normality Result (a = 0.05)		Pass
Critical Value		8.42E-01	Calculated Value for dataset		8.80E-01
Anderson Darling (AD) A^2		5.55E-01	AD Probability	Pass	6.91E-01
90% UCL of the MVUE		2.11E+05	95% UCL of the MVUE		2.22E+05
Jackknife Results					
Jackknifed Mean		1.79E+05	Jackknifed Standard Error		1.60E+04
90% UCL of the mean		2.02E+05	95% UCL of the mean		2.09E+05
90% UCL of the $MVUE^2$		2.03E+05	95% UCL of the $MVUE^2$		2.10E+05

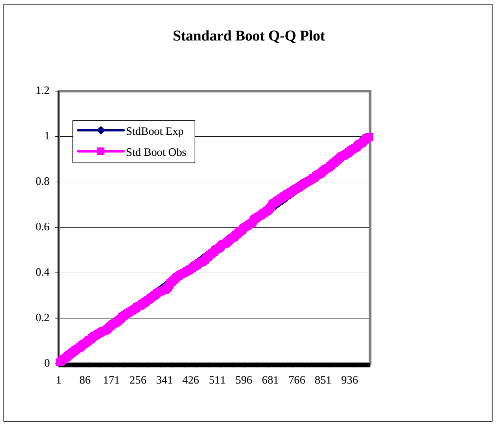
Bootstrap Results (Raw Data)						
Standard Bootstrap	Mean	1.79E+05	90% UCL	1.98E+05	95% UCL	2.03E+05
	Skewness	5.37E-02	Kurtosis	2.99E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Pivitol (t) Bootstrap	90% UCL	2.00E+05	95% UCL	2.06E+05		
	Skewness	1.19E+00	Kurtosis	9.29E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Hall's t Bootstrap	90% UCL	1.98E+05	95% UCL	2.06E+05		
	Skewness	3.34E-01	Kurtosis	8.40E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						

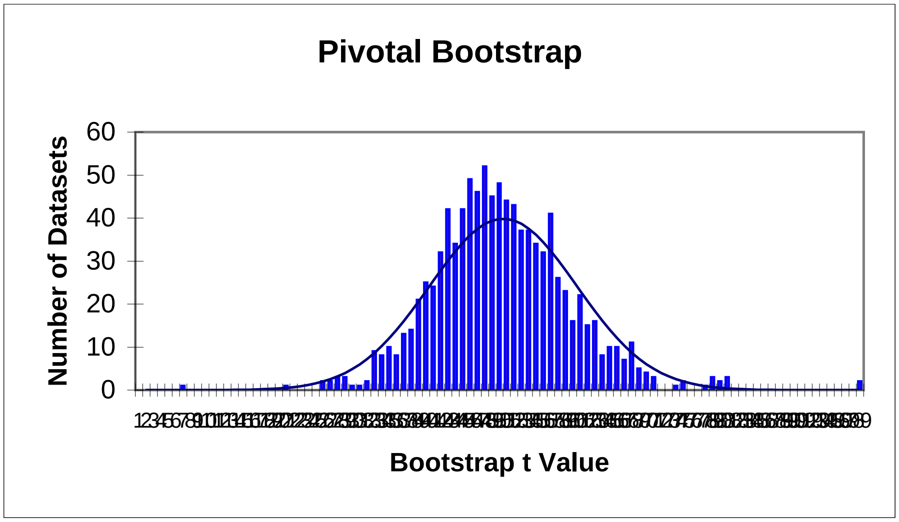
2 = Using the Jackknife

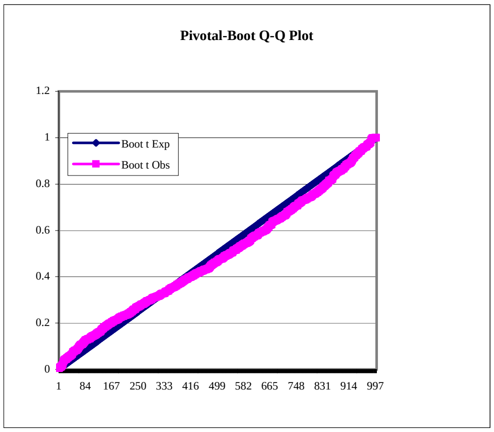
MVUE=Minimum Variance Unbiased Estimator
UCL=Upper Confidence Interval

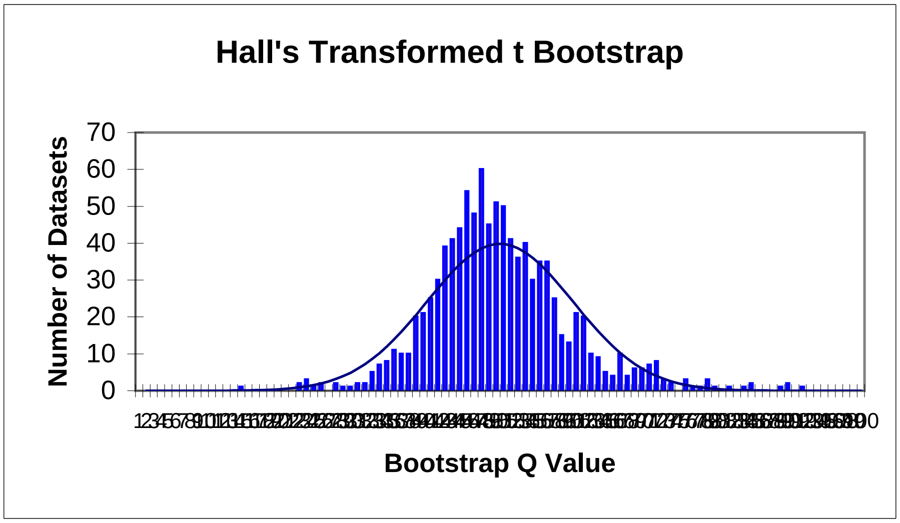
BOOTSTRAP RESULTS FOR OCTANOL-WATER PARTITIONING COEFFCIENTS FOR DICHLOROBIPHENYLS OBTAINED FROM EISLER AND BELISLE (1996)

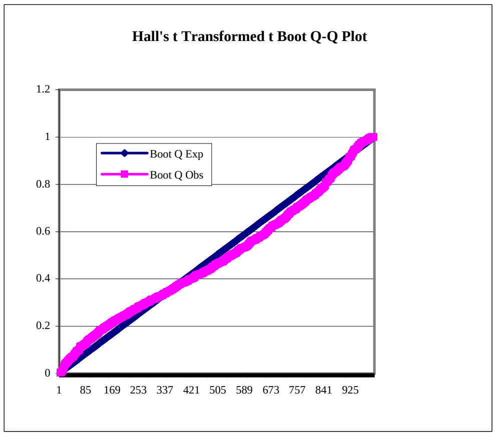












STATISTICAL ANALYSIS OF OCTANOL-WATER PARTITIONING COEFFICIENTS OBTAINED FROM EISLER AND BELISLE (1996)

Trichlorobiphenyls

The data are best described as normally distributed and there were a sufficient number of detected values to perform a statistical analysis.

Congener	Value	$Log_{10}Kow$
16	204644	5.311
17	576766	5.761
18	355631	5.551
19	302691	5.481
20	377572	5.577
21	147911	5.170
22	263633	5.421
23	377572	5.577
24	468813	5.671
25	475335	5.677
26	464515	5.667
27	279898	5.447
28	490908	5.691
29	553350	5.743
30	319154	5.504
31	475335	5.677
32	563638	5.751
33	373250	5.572
34	464515	5.667
35	671429	5.827
36	14158	4.151
37	87297	4.941
38	584790	5.767
39	788860	5.897

Recommended Mean	Normal Mean	403403	Log_{10}	5.606
Recommended UCL	UCL based on t-statistic	467582	Log_{10}	5.670

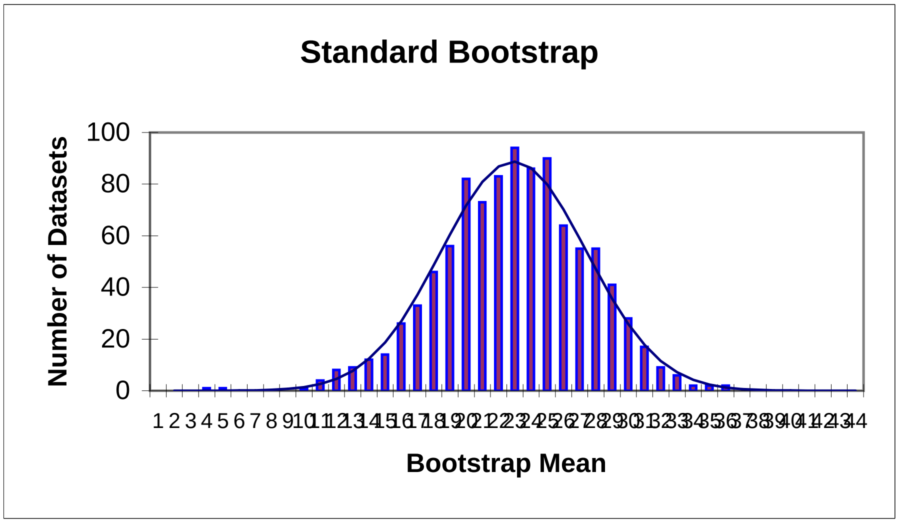
Raw Data Results					
Number of Values		24			
Maximum Value		7.89E+05	Minimum Value		1.42E+04
Normal (Non-transformed) Results					
Normal Mean		4.03E+05	Mean Standard Error		3.74E+04
Standard Deviation		1.83E+05	Coefficient of Variance (%)		45%
Dataset Skewness	Pass	-1.63E-01	Dataset Kurtosis	Pass	2.58E+00
Tested for Normality		W-Test	NormalityResult (a = 0.05)		Pass
Critical Value		9.16E-01	Calculated Value for datasei		9.85E-01
90% UCL using t-statistic		4.53E+05	95% UCL using -t-statistic		4.68E+05
Natural Log-Transformed Results					
MVUE of the log-mean		4.60E+05	Standard error of the log-me		8.60E+04
Standard Deviation		8.32E-01	Coefficient of Variance (%)		7%
Dataset Skewness	Fail	-2.3E+00	Dataset Kurtosis	Fail	9.02E+00
Tested for Normality		W-Test	Normality Result (a = 0.05)		Fail
Critical Value		9.16E-01	Calculated Value for datasei		7.23E-01
Anderson Darling (AD) A^2		2.03E+00	AD Probability	Fail	8.82E-02
90% UCL of the MVUE		6.31E+05	95% UCL of the MVUE		6.99E+05
Jackknife Results					
Jackknifed Mean		4.03E+05	Jackknifed Standard Error		3.74E+04
90% UCL of the mean		4.53E+05	95% UCL of the mean		4.68E+05
90% UCL of the MVUE[2]		5.35E+05	95% UCL of the MVUE[2]		5.55E+05

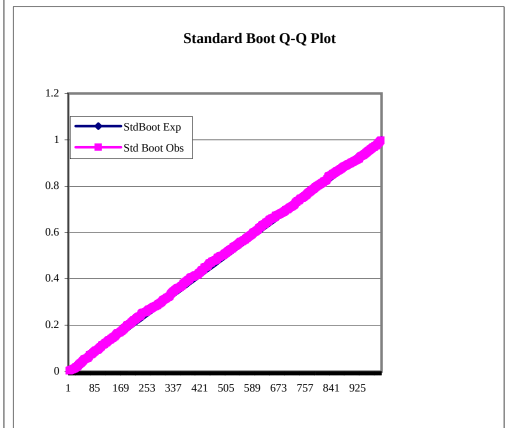
Bootstrap Results (Raw Data)						
Standard Bootstrap	Mean	4.02E+05	90% UCL	4.48E+05	95% UCL	4.61E+05
Skewness	-2.19E-01		Kurtosis	3.25E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Pivitol (t) Bootstrap	90% UCL	4.52E+05	95% UCL	4.71E+05		
Skewness	-1.48E-01		Kurtosis	3.65E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Hall's t Bootstrap	90% UCL	4.53E+05	95% UCL	4.73E+05		
Skewness	-9.08E-02		Kurtosis	4.21E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						

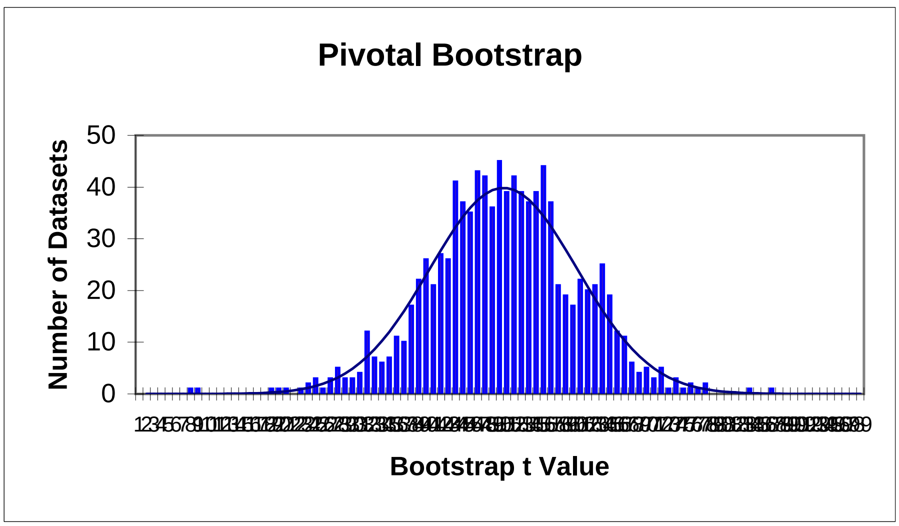
2 = Using the Jackknife

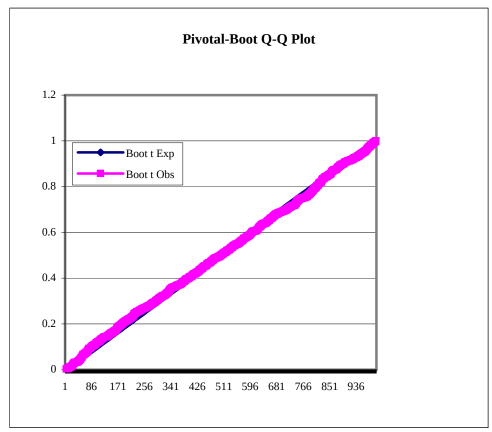
MVUE=Minimum Variance Unbiased Estimator
UCL=Upper Confidence Interval

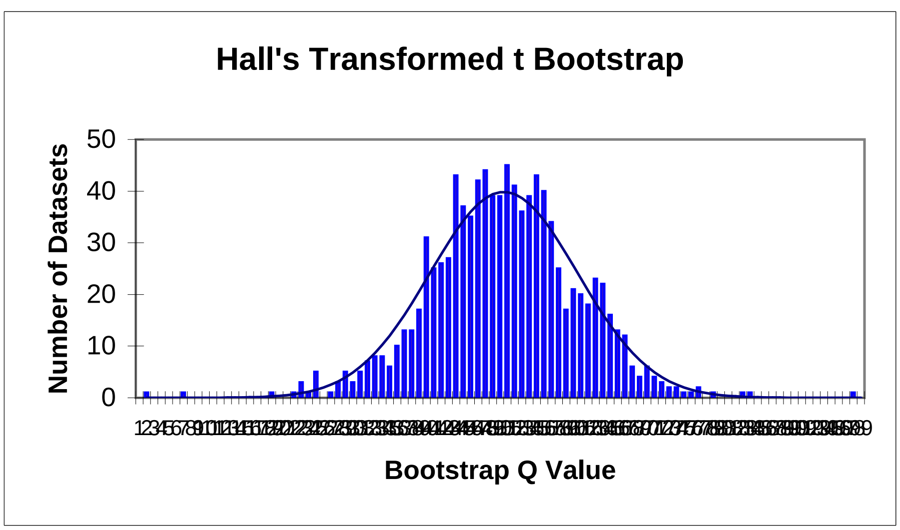
BOOTSTRAP RESULTS FOR OCTANOL-WATER PARTITIONING COEFFCIENTS FOR TRICHLOROBIPHENYLS OBTAINED FROM EISLER AND BELISLE (1996)

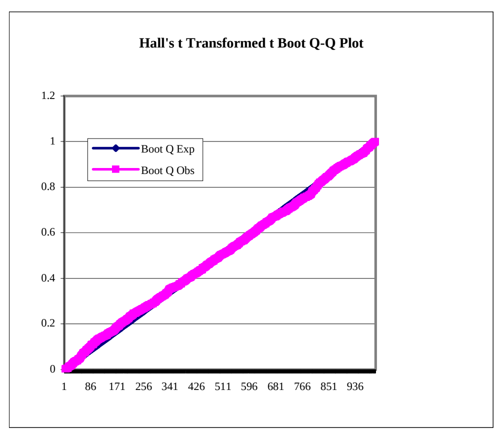












STATISTICAL ANALYSIS OF OCTANOL-WATER PARTITIONING COEFFICIENTS OBTAINED FROM EISLER AND BELISLE (1996)

Tetrachlorobiphenyls

The data are best described as log-normally distributed and there were a sufficient number of detected values to perform statistical analysis. The CV is less than 100%

Recommended Mean	MVUE of the log-mean	1330250	Log_{10}	6.124
Recommended UCL	UCL based on H-statistic	1683184	Log_{10}	6.226

Congener	Value	$Log_{10}Kow$
40	363915	5.561
41	1291219	6.111
42	584790	5.767
43	571479	5.757
44	647143	5.811
45	344350	5.537
46	344350	5.537
47	1954339	6.291
48	612350	5.787
49	1663413	6.221
50	433511	5.637
51	433511	5.637
52	1233105	6.091
53	423643	5.627
54	801678	5.904
55	1309182	6.117
56	1309182	6.117
57	1503142	6.177
58	1503142	6.177
59	905733	5.957
60	283139	5.452
61	877001	5.943
62	788860	5.897
63	1503142	6.177
64	905733	5.957
65	736207	5.867
66	283139	5.452
67	1610646	6.207
68	1849269	6.267
69	1114295	6.047
70	1702159	6.231
71	970510	5.987
72	1849269	6.267
73	1114295	6.047
74	4688134	6.671
75	1140250	6.057
76	1370882	6.137
77	3334264	6.523
78	2275097	6.357
79	2673006	6.427
80	3828247	6.583
81	2328091	6.367

Raw Data Results

Number of Values	42		
Maximum Value	4.69E+06	Minimum Value	2.83E+05

Normal (Non-transformed) Results

Normal Mean		1.32E+06	Mean Standard Error		1.48E+05
Standard Deviation		9.62E+05	Coefficient of Variance (%)		73%
Dataset Skewness	Fail	1.55E+00	Dataset Kurtosis	Fail	5.52E+00
Tested for Normality		W-Test	NormalityResult (a = 0.05)		Fail
Critical Value		9.42E-01	Calculated Value for dataset		8.51E-01
90% UCL using t-statistic		1.51E+06	95% UCL using -t-statistic		1.57E+06

Natural Log-Transformed Results

MVUE of the log-mean		1.33E+06	Standard error of the log-me		1.59E+05
Standard Deviation		7.10E-01	Coefficient of Variance (%)		5%
Dataset Skewness	Pass	-6.40E-02	Dataset Kurtosis	Pass	2.27E+00
Tested for Normality		W-Test	Normality Result (a = 0.05)		Pass
Critical Value		9.42E-01	Calculated Value for dataset		9.71E-01
Anderson Darling (AD) A^2		2.77E-01	AD Probability	Pass	9.54E-01
90% UCL of the MVUE		1.59E+06	95% UCL of the MVUE		1.68E+06

Jackknife Results

Jackknifed Mean	1.32E+06	Jackknifed Standard Error	1.48E+05
90% UCL of the mean	1.51E+06	95% UCL of the mean	1.57E+06
90% UCL of the MVUE[2]	1.53E+06	95% UCL of the MVUE[2]	1.59E+06

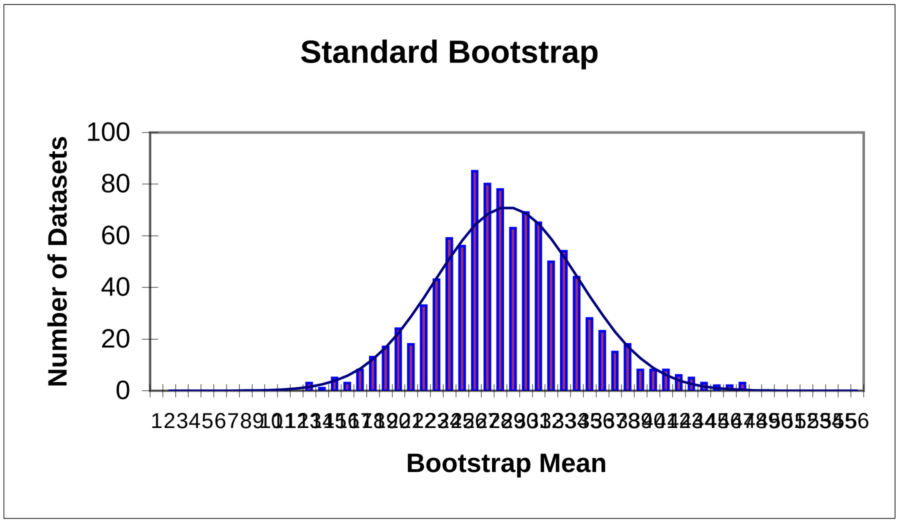
Bootstrap Results (Raw Data)

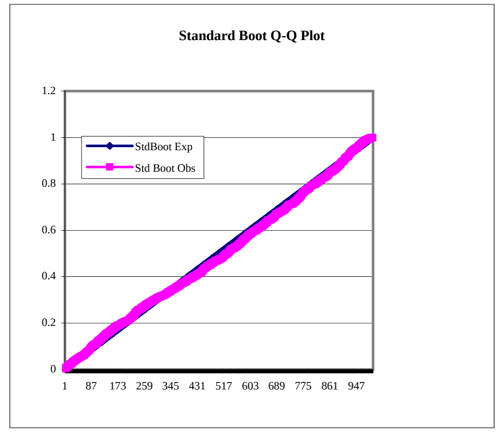
Standard Bootstrap	Mean	1.32E+06	90% UCL	1.52E+06	95% UCL	1.57E+06
Skewness	2.88E-01		Kurtosis	3.39E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Pivitol (t) Bootstrap	90% UCL	1.54E+06	95% UCL			1.62E+06
Skewness	-6.83E-01		Kurtosis	4.57E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Hall's t Bootstrap	90% UCL	1.54E+06	95% UCL			1.61E+06
Skewness	########		Kurtosis	5.78E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						

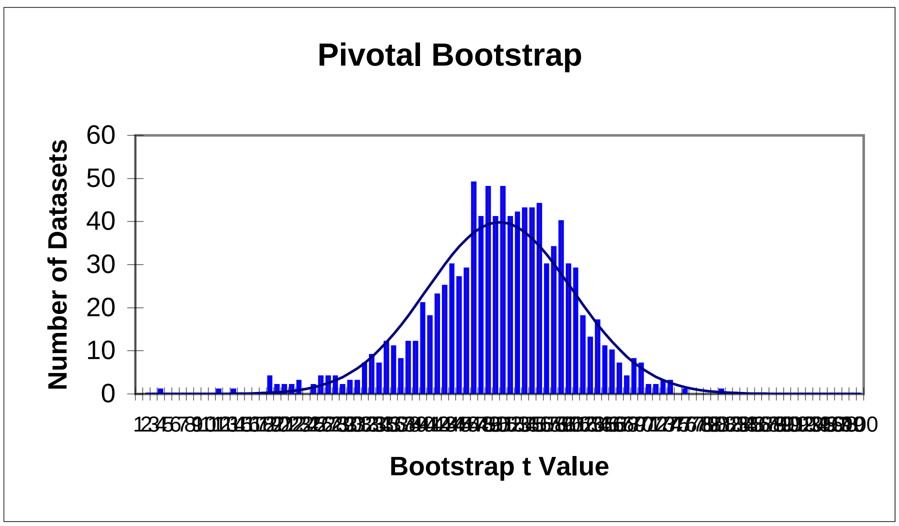
2 = Using the Jackknife

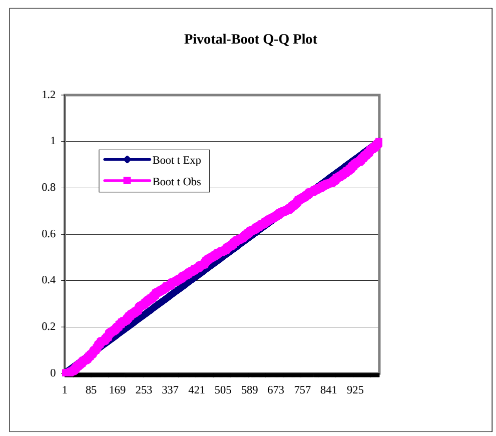
MVUE=Minimum Variance Unbiased Estimator
UCL=Upper Confidence Interval

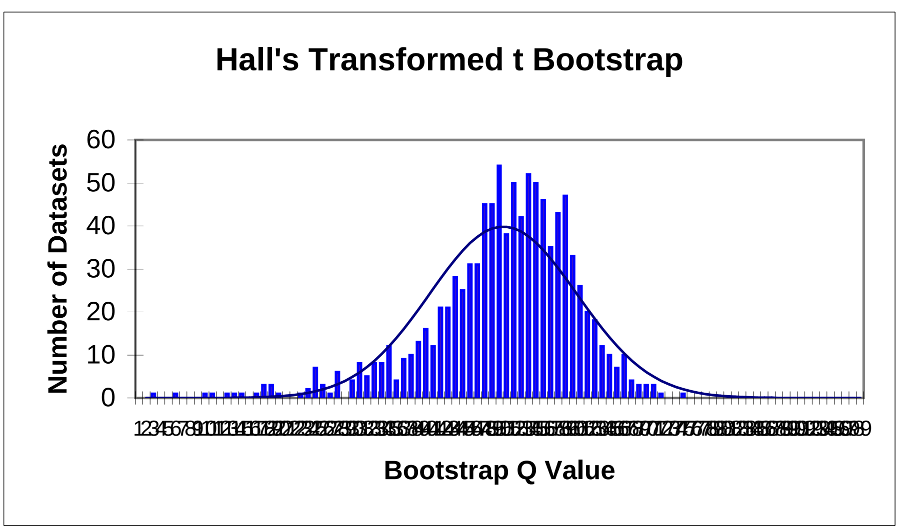
BOOTSTRAP RESULTS FOR OCTANOL-WATER PARTITIONING COEFFCIENTS FOR TETRACHLOROBIPHENYLS OBTAINED FROM EISLER AND BELISLE (1996)

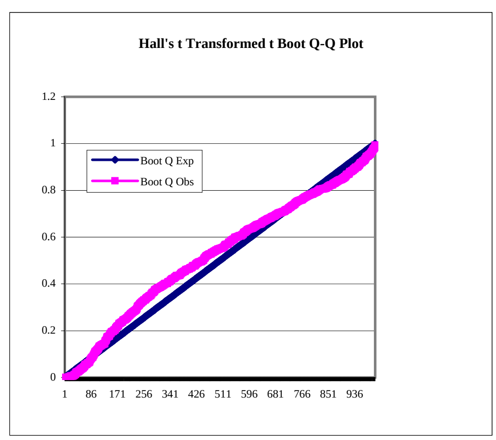












STATISTICAL ANALYSIS OF OCTANOL-WATER PARTITIONING COEFFICIENTS OBTAINED FROM EISLER AND BELISLE (1996)

Pentachlorobiphenyls

The data are best described as log-normally distributed and there were a sufficient number of detected values to perform statistical analysis. The CV is > 100%

Congener	Value	$Log_{10}Kow$
82	1386756	6.142
83	1849269	6.267
84	1099006	6.041
85	4083194	6.611
86	1599558	6.204
87	2349633	6.371
88	32809529	7.516
89	1193988	6.077
90	2328091	6.367
91	1370882	6.137
92	2275097	6.357
93	1114295	6.047
94	1370882	6.137
95	1370882	6.137
96	521195	5.717
97	4688134	6.671
98	1370882	6.137
99	16255488	7.211
100	1725838	6.237
101	11776060	7.071
102	1468926	6.167
103	1686553	6.227
104	656145	5.817
105	4539416	6.657
106	4436086	6.647
107	5211947	6.717
108	5211947	6.717
109	3069022	6.487
110	3404082	6.532
111	5847901	6.767
112	2864178	6.457
113	3523709	6.547
114	4539416	6.657
115	3140509	6.497
116	2013724	6.304
117	2930893	6.467
118	13212956	7.121
119	3863670	6.587
120	6266139	6.797
121	4436086	6.647
122	4436086	6.647
123	5584702	6.747
124	5457579	6.737
125	3288516	6.517
126	7888601	6.897
127	9057326	6.957

Recommended Mean	MVUE of the log-mean	4400776	Log_{10}	6.644
Recommended UCL	UCL based on Jackknifed MVUE	5544897	Log_{10}	6.744

Raw Data Results

Number of Values	46			
Maximum Value	3.28E+07	Minimum Value		5.21E+05

Normal (Non-transformed) Results

Normal Mean		4.58E+06	Mean Standard Error		7.91E+05
Standard Deviation		5.37E+06	Coefficient of Variance (%)		117%
Dataset Skewness	Fail	3.47E+00	Dataset Kurtosis	Fail	1.74E+01
Tested for Normality		W-Test	NormalityResult (a = 0.05)		Fail
Critical Value		9.45E-01	Calculated Value for dataset		6.19E-01
90% UCL using t-statistic		5.61E+06	95% UCL using -t-statistic		5.91E+06

Natural Log-Transformed Results

MVUE of the log-mean		4.40E+06	Standard error of the log-me		6.14E+05
Standard Deviation		8.39E-01	Coefficient of Variance (%)		6%
Dataset Skewness	Pass	3.45E-01	Dataset Kurtosis	Pass	3.11E+00
Tested for Normality		W-Test	Normality Result (a = 0.05)		Pass
Critical Value		9.45E-01	Calculated Value for dataset		9.79E-01
Anderson Darling (AD) A^2		3.48E-01	AD Probability	Pass	8.99E-01
90% UCL of the MVUE		5.46E+06	95% UCL of the MVUE		5.82E+06

Jackknife Results

Jackknifed Mean	4.58E+06	Jackknifed Standard Error	7.91E+05
90% UCL of the mean	5.61E+06	95% UCL of the mean	5.91E+06
90% UCL of the MVUE[2]	5.28E+06	95% UCL of the MVUE[2]	5.54E+06

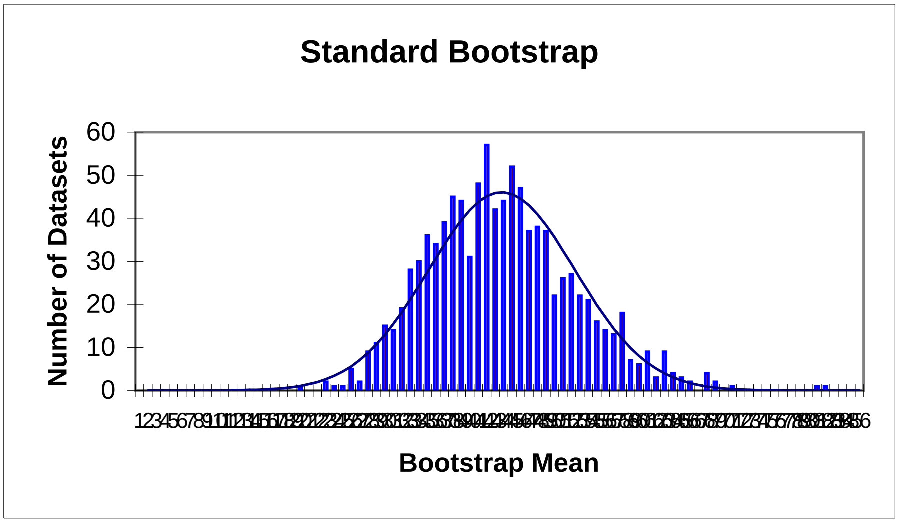
Bootstrap Results (Raw Data)

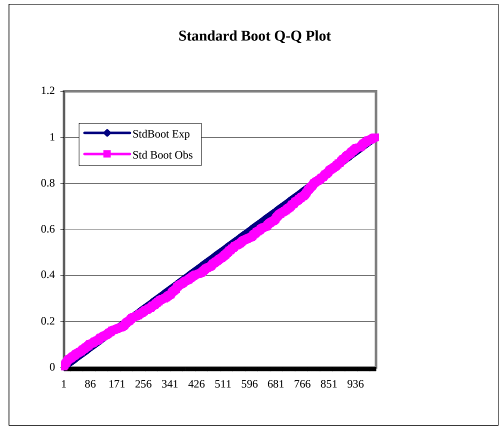
Standard Bootstrap	Mean	4.57E+06	90% UCL	5.58E+06	95% UCL	5.87E+06
	Skewness	4.76E-01	Kurtosis	3.43E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Pivitol (t) Bootstrap	90% UCL	6.39E+06	95% UCL	7.10E+06		
	Skewness	-1.6E+00	Kurtosis	7.30E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Hall's t Bootstrap	90% UCL	6.52E+06	95% UCL	7.20E+06		
	Skewness	-2.6E+00	Kurtosis	1.58E+01		
Quantile fit is poor do not use Bootstrap Results						

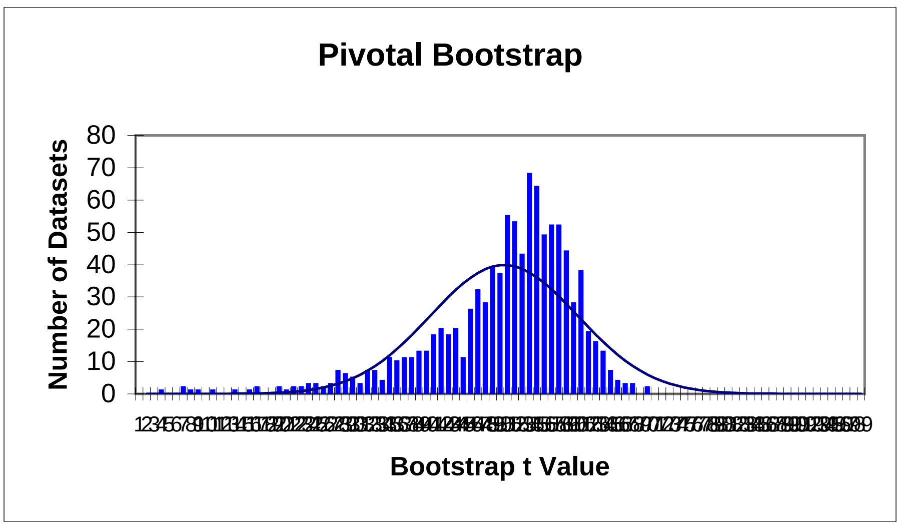
2 = Using the Jackknife

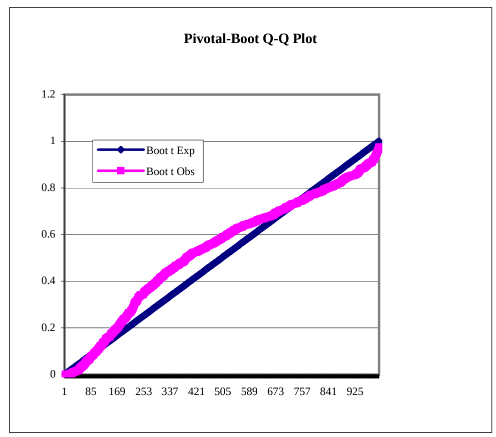
MVUE=Minimum Variance Unbiased Estimator
UCL=Upper Confidence Interval

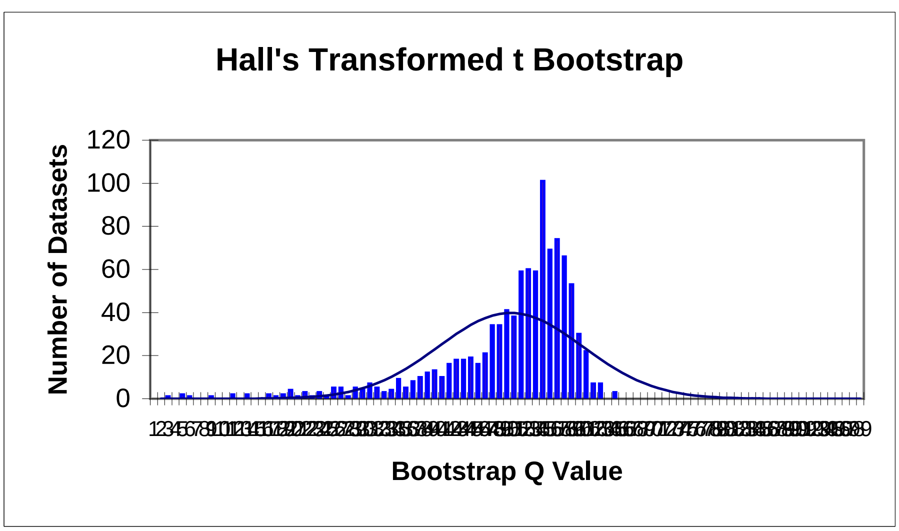
BOOTSTRAP RESULTS FOR OCTANOL-WATER PARTITIONING COEFFCIENTS FOR PENTACHLOROBIPHENYLS OBTAINED FROM EISLER AND BELISLE (1996)

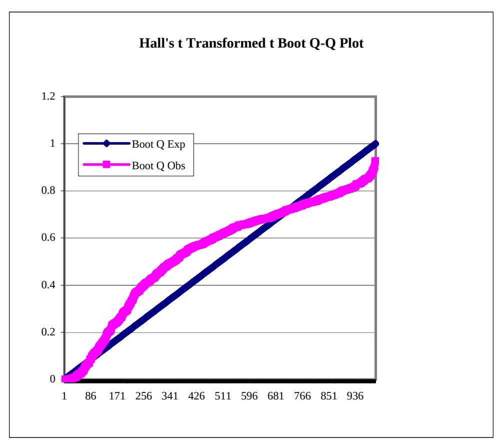












STATISTICAL ANALYSIS OF OCTANOL-WATER PARTITIONING COEFFICIENTS OBTAINED FROM EISLER AND BELISLE (1996)

Hexachlorobiphenyls

The data are best described as log-normally distributed and there were a sufficient number of detected values to perform statistical analysis. The CV is less than 100%

Congener	Value	$Log_{10}Kow$
128	9141132	6.961
129	20941125	7.321
130	24603676	7.391
131	3863670	6.587
132	3863670	6.587
133	7362071	6.867
134	20137242	7.304
135	14157938	7.151
136	3243396	6.511
137	51404365	7.711
138	27605779	7.441
139	4753352	6.677
140	4753352	6.677
141	39084090	7.592
142	3288516	6.517
143	4045759	6.607
144	4753352	6.677
145	1807174	6.257
146	7888601	6.897
147	4436086	6.647
148	5457579	6.737
149	19098533	7.281
150	2123244	6.327
151	4436086	6.647
152	1686553	6.227
153	56363766	7.751
154	5847901	6.767
155	13273945	7.123
156	15381546	7.187
157	15381546	7.187
158	10641430	7.027
159	17660378	7.247
160	8649679	6.937
161	12217997	7.087
162	17660378	7.247
163	9931160	6.997
164	10641430	7.027
165	11402498	7.057
166	8649679	6.937
167	18923436	7.277
168	13091819	7.117
169	26730064	7.427

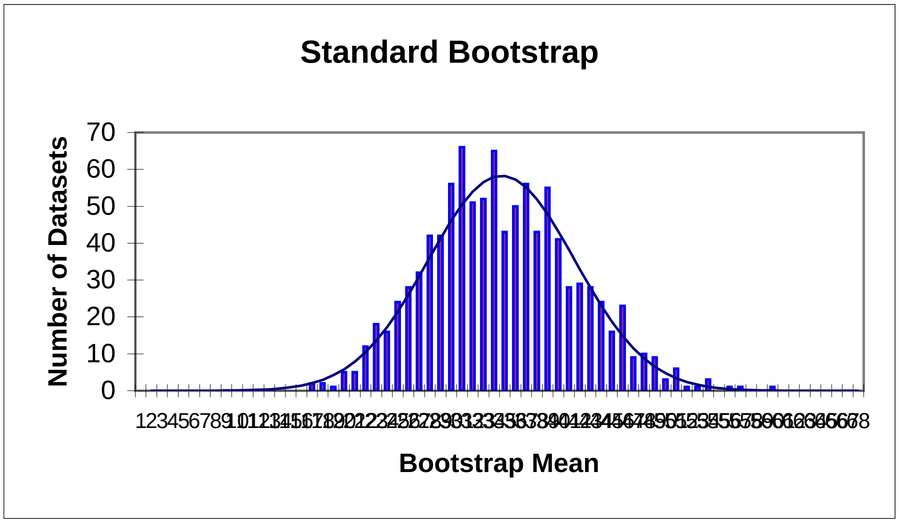
Recommended Mean	MVUE of the log-mean	13630937	Log_{10}	7.135
Recommended UCL	UCL based on H-statistic	18596711	Log_{10}	7.269

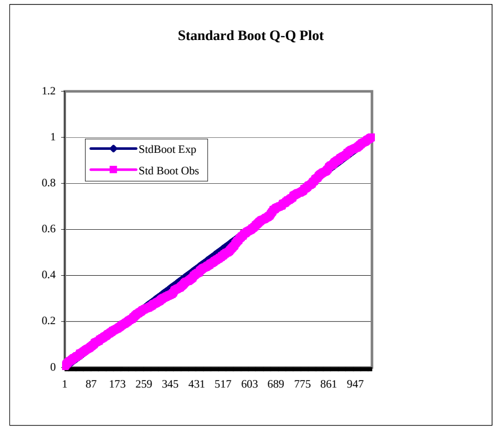
Raw Data Results					
Number of Values		42			
Maximum Value		5.64E+07	Minimum Value		1.69E+06
Normal (Non-transformed) Results					
Normal Mean		1.35E+07	Mean Standard Error		1.90E+06
Standard Deviation		1.23E+07	Coefficient of Variance (%)		91%
Dataset Skewness	Fail	1.83E+00	Dataset Kurtosis	Fail	6.35E+00
Tested for Normality		W-Test	NormalityResult (a = 0.05)		Fail
Critical Value		9.42E-01	Calculated Value for datase		7.91E-01
90% UCL using t-statistic		1.60E+07	95% UCL using -t-statistic		1.67E+07
Natural Log-Transformed Results					
MVUE of the log-mean		1.36E+07	Standard error of the log-me		2.07E+06
Standard Deviation		8.68E-01	Coefficient of Variance (%)		5%
Dataset Skewness	Pass	-2.00E-02	Dataset Kurtosis	Pass	2.29E+00
Tested for Normality		W-Test	Normality Result (a = 0.05)		Pass
Critical Value		9.42E-01	Calculated Value for datase		9.76E-01
Anderson Darling (AD) A^2		2.41E-01	AD Probability	Pass	9.75E-01
90% UCL of the MVUE		1.73E+07	95% UCL of the MVUE		1.86E+07
Jackknife Results					
Jackknifed Mean		1.35E+07	Jackknifed Standard Error		1.90E+06
90% UCL of the mean		1.60E+07	95% UCL of the mean		1.67E+07
90% UCL of the MVUE[2]		1.62E+07	95% UCL of the MVUE[2]		1.70E+07

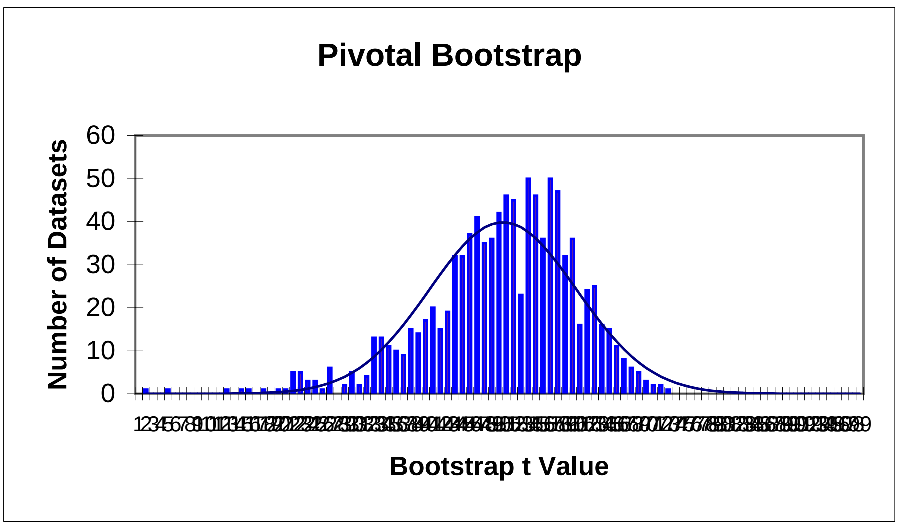
Bootstrap Results (Raw Data)							
Standard Bootstrap	Mean	1.35E+07	90% UCL	1.59E+07	95% UCL	1.65E+07	
Skewness	2.54E-01		Kurtosis	2.89E+00			
Quantile fit is good - Bootstrap Output is Normal or nearly so							
Pivitol (t) Bootstrap	90% UCL	1.66E+07		95% UCL		1.76E+07	
Skewness	-8.04E-01		Kurtosis	4.27E+00			
Quantile fit is good - Bootstrap Output is Normal or nearly so							
Hall's t Bootstrap	90% UCL	1.65E+07		95% UCL		1.82E+07	
Skewness	-1.3E+00		Kurtosis	6.13E+00			
Quantile fit is good - Bootstrap Output is Normal or nearly so							

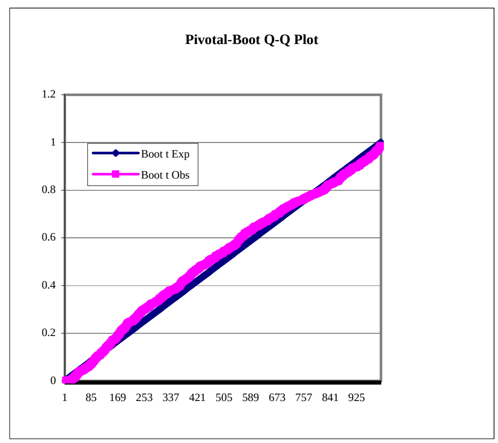
MVUE=Minimum Variance Unbiased Estimator
2 = Using the Jackknife
UCL=Upper Confidence Interval

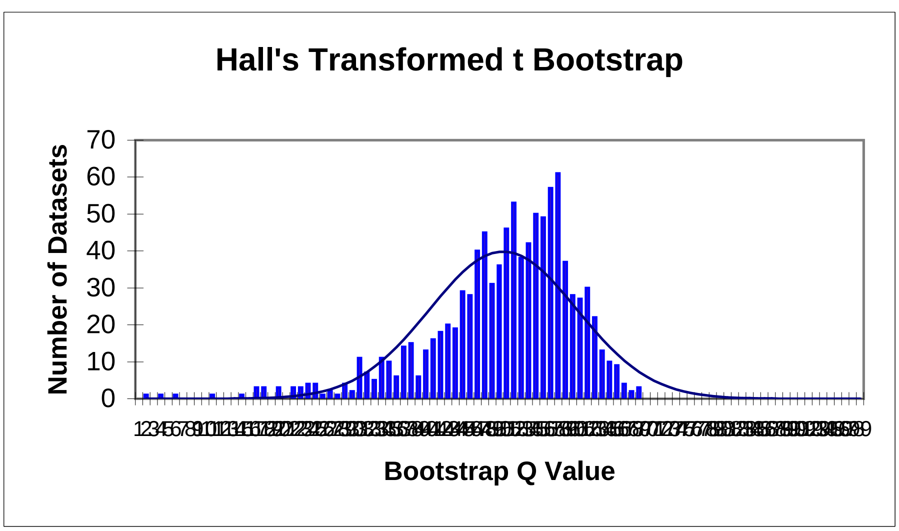
BOOTSTRAP RESULTS FOR OCTANOL-WATER PARTITIONING COEFFCIENTS FOR HEXACHLOROBIPHENYLS OBTAINED FROM EISLER AND BELISLE (1996)

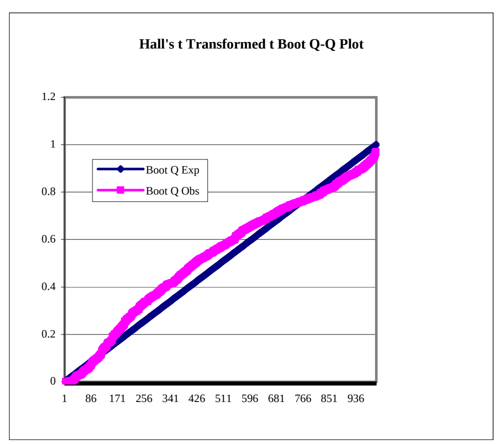












STATISTICAL ANALYSIS OF OCTANOL-WATER PARTITIONING COEFFICIENTS OBTAINED FROM EISLER AND BELISLE (1996)

Heptachlorobiphenyls

The data are best described as log-normally distributed and there were a sufficient number of detected values to perform statistical analysis. The CV is less than 100%

Congener	Value	$Log_{10}Kow$
170	18923436	7.277
171	5058247	6.704
172	21727012	7.337
173	10641430	7.027
174	13091819	7.117
175	15031420	7.177
176	5847901	6.767
177	12217997	7.087
178	14028137	7.147
179	5457579	6.737
180	23280913	7.367
181	13091819	7.117
182	16106456	7.207
183	16106456	7.207
184	7194490	6.857
185	85703785	7.933
186	4977371	6.697
187	15031420	7.177
188	6714289	6.827
189	52119471	7.717
190	29308932	7.467
191	36057864	7.557
192	33651157	7.527
193	33651157	7.527

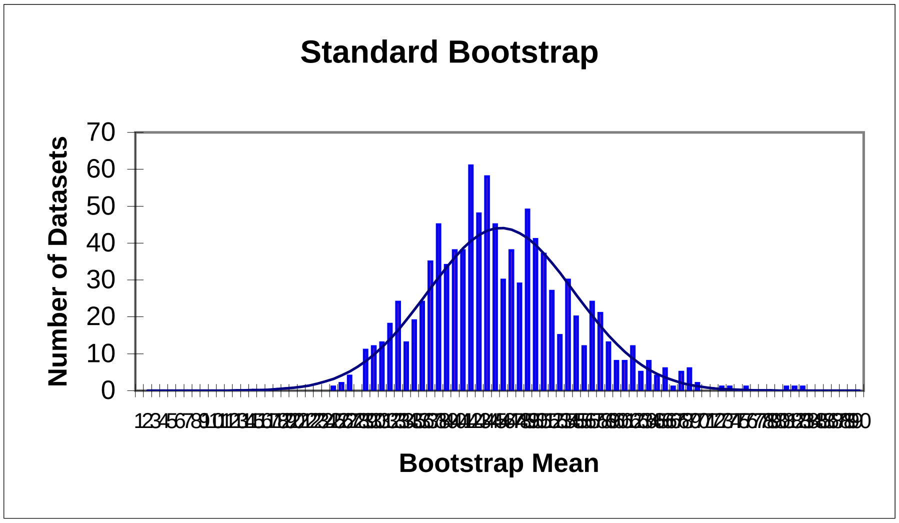
Recommended Mean	MVUE of the log-mean	20323408	Log_{10}	7.308
Recommended UCL	UCL based on H-statistic	29257630	Log_{10}	7.466

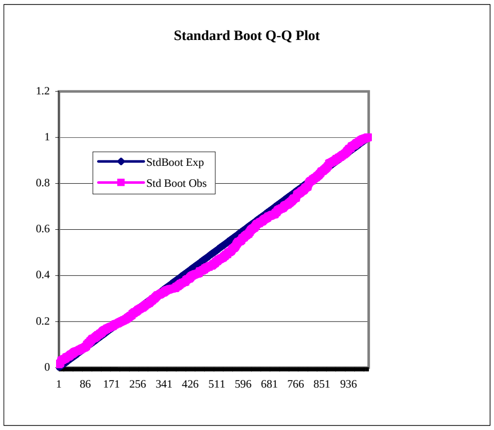
Raw Data Results					
Number of Values		24			
Maximum Value		8.57E+07	Minimum Value		4.98E+06
Normal (Non-transformed) Results					
Normal Mean		2.06E+07	Mean Standard Error		3.72E+06
Standard Deviation		1.82E+07	Coefficient of Variance (%)		88%
Dataset Skewness	Fail	2.02E+00	Dataset Kurtosis	Fail	7.33E+00
Tested for Normality		W-Test	NormalityResult (a = 0.05)		Fail
Critical Value		9.16E-01	Calculated Value for datase		7.58E-01
90% UCL using t-statistic		2.55E+07	95% UCL using -t-statistic		2.70E+07
Natural Log-Transformed Results					
MVUE of the log-mean		2.03E+07	Standard error of the log-me		3.41E+06
Standard Deviation		7.57E-01	Coefficient of Variance (%)		5%
Dataset Skewness	Pass	2.56E-01	Dataset Kurtosis	Pass	2.33E+00
Tested for Normality		W-Test	Normality Result (a = 0.05)		Pass
Critical Value		9.16E-01	Calculated Value for datase		9.62E-01
Anderson Darling (AD) A^2		2.91E-01	AD Probability	Pass	9.45E-01
90% UCL of the MVUE		2.68E+07	95% UCL of the MVUE		2.93E+07
Jackknife Results					
Jackknifed Mean		2.06E+07	Jackknifed Standard Error		3.72E+06
90% UCL of the mean		2.55E+07	95% UCL of the mean		2.70E+07
90% UCL of the MVUE[2]		2.51E+07	95% UCL of the MVUE[2]		2.65E+07
Bootstrap Results (Raw Data)					
Standard Bootstrap	Mean	2.05E+07	90% UCL	2.52E+07	95% UCL 2.66E+07
Skewness	5.50E-01		Kurtosis	3.48E+00	
Quantile fit is good - Bootstrap Output is Normal or nearly so					
Pivitol (t) Bootstrap	90% UCL	2.87E+07	95% UCL		3.19E+07
Skewness	-1.2E+00		Kurtosis	5.69E+00	
Quantile fit is good - Bootstrap Output is Normal or nearly so					
Hall's t Bootstrap	90% UCL	2.92E+07	95% UCL		3.25E+07
Skewness	-1.8E+00		Kurtosis	7.95E+00	
Quantile fit is poor do not use Bootstrap Results					

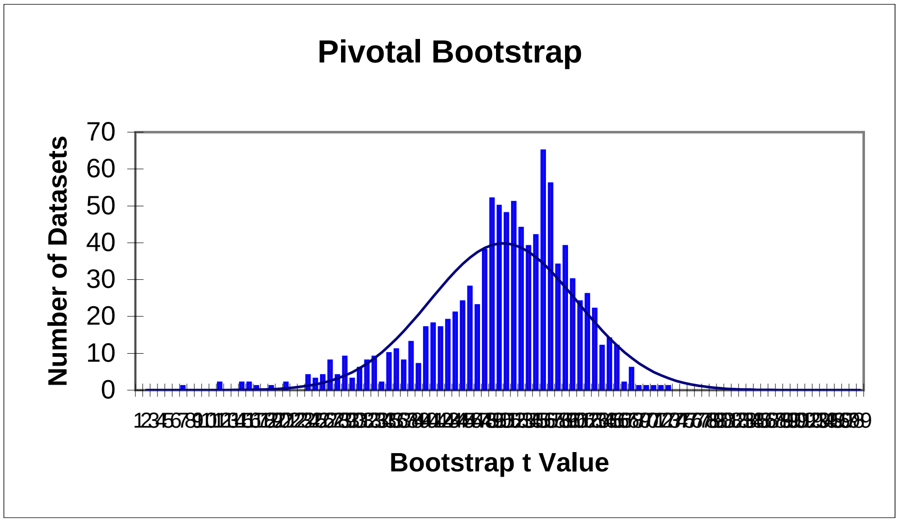
2 = Using the Jackknife

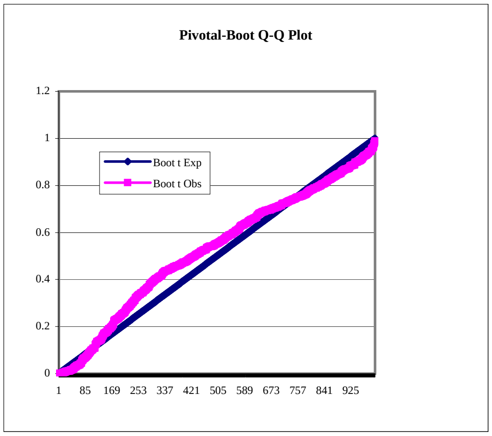
MVUE=Minimum Variance Unbiased Estimator
UCL=Upper Confidence Interval

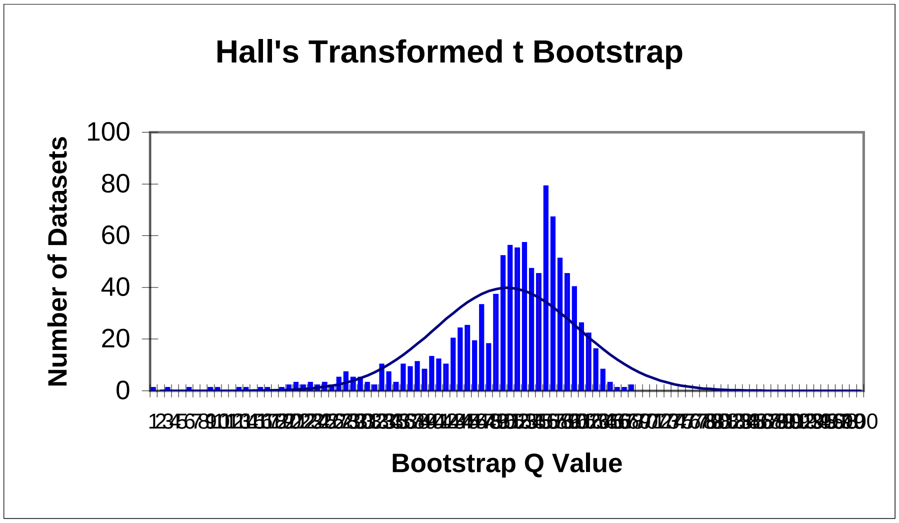
BOOTSTRAP RESULTS FOR OCTANOL-WATER PARTITIONING COEFFCIENTS FOR HEPTACHLOROBIPHENYLS OBTAINED FROM EISLER AND BELISLE (1996)

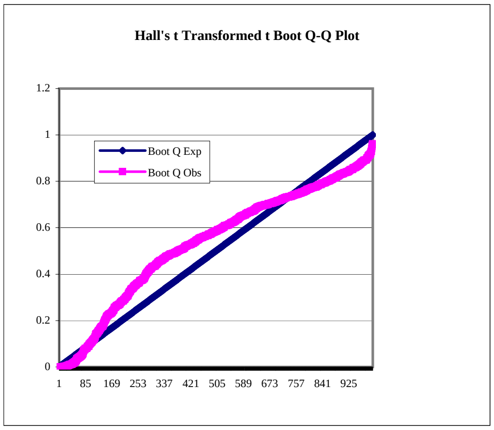












STATISTICAL ANALYSIS OF OCTANOL-WATER PARTITIONING COEFFICIENTS OBTAINED FROM EISLER AND BELISLE (1996)

Octachlorobiphenyls

There is a sufficient number of values for statistical analysis - the data were found to be non-normally distributed and the number of samples is below 15

Congener	Value	$Log_{10}Kow$
194	481947798	8.683
195	36897760	7.567
196	45394162	7.657
197	20276827	7.307
198	42364297	7.627
199	16106456	7.207
200	18923436	7.277
201	42364297	7.627
202	264850014	8.423
203	45394162	7.657
204	20276827	7.307
205	101624869	8.007

Recommended Mean	Jackknife Mean	94701742	Log_{10}	7.976
Recommended UCL	Jackknifed UCL	167287874	Log_{10}	8.223

Raw Data Results					
Number of Values		12			
Maximum Value		4.82E+08	Minimum Value		1.61E+07
Normal (Non-transformed) Results					
Normal Mean		9.47E+07	Mean Standard Error		4.04E+07
Standard Deviation		1.40E+08	Coefficient of Variance (%)		148%
Dataset Skewness	Fail	1.84E+00	Dataset Kurtosis	Pass	5.10E+00
Tested for Normality		W-Test	NormalityResult (a = 0.05)		Fail
Critical Value		8.59E-01	Calculated Value for dataset		6.03E-01
90% UCL using t-statistic		1.50E+08	95% UCL using -t-statistic		1.67E+08
Natural Log-Transformed Results					
MVUE of the log-mean		8.17E+07	Standard error of the log-me		2.70E+07
Standard Deviation		1.06E+00	Coefficient of Variance (%)		6%
Dataset Skewness	Pass	9.04E-01	Dataset Kurtosis	Pass	2.52E+00
Tested for Normality		W-Test	Normality Result (a = 0.05)		Fail
Critical Value		8.59E-01	Calculated Value for dataset		8.56E-01
Anderson Darling (AD) A^2		7.38E-01	AD Probability	Pass	5.27E-01
90% UCL of the MVUE		1.74E+08	95% UCL of the MVUE		2.31E+08
Jackknife Results					
Jackknifed Mean		9.47E+07	Jackknifed Standard Error		4.04E+07
90% UCL of the mean		1.50E+08	95% UCL of the mean		1.67E+08
90% UCL of the MVUE[2]		1.26E+08	95% UCL of the MVUE[2]		1.42E+08

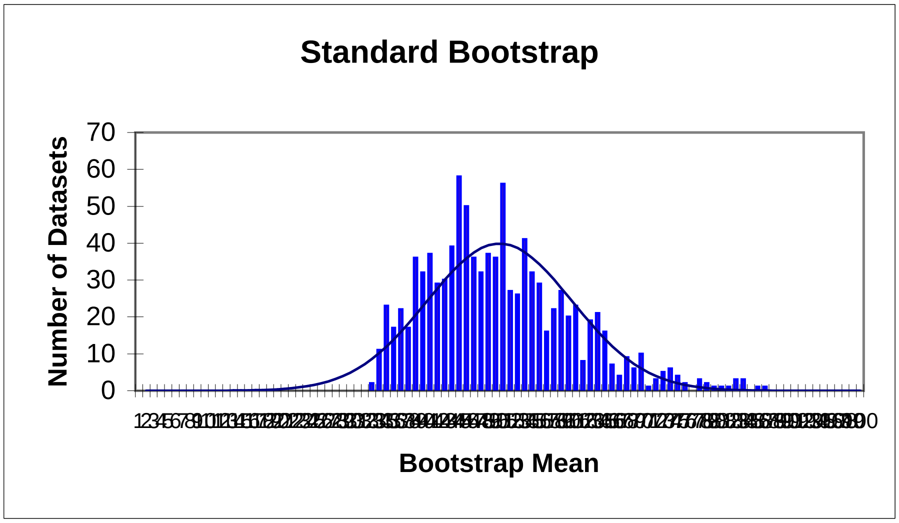
Bootstrap Results (Raw Data)						
Standard Bootstrap	Mean	9.48E+07	90% UCL	1.46E+08	95% UCL	1.60E+08
Skewness	7.41E-01		Kurtosis	3.45E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Pivitol (t) Bootstrap	90% UCL	2.95E+08		95% UCL		4.52E+08
Skewness	-3.4E+00		Kurtosis	1.52E+01		
Quantile fit is poor do not use Bootstrap Results						
Hall's t Bootstrap	90% UCL	2.92E+08		95% UCL		3.58E+08
Skewness	-4.8E+00		Kurtosis	3.49E+01		
Quantile fit is poor do not use Bootstrap Results						

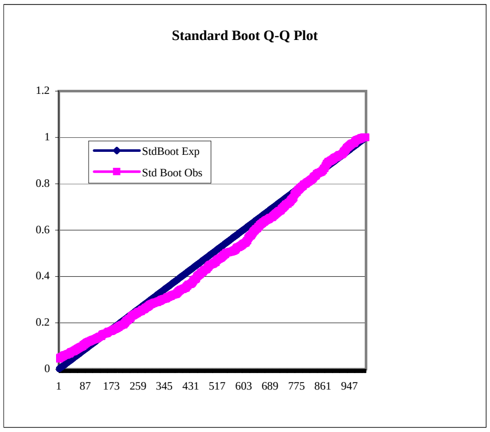
MVUE=Minimum Variance Unbiased Estimator

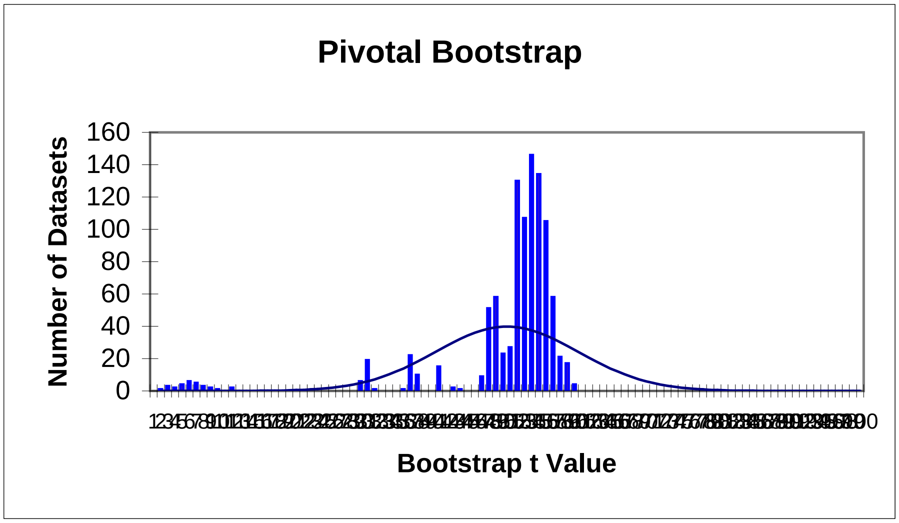
2 = Using the Jackknife

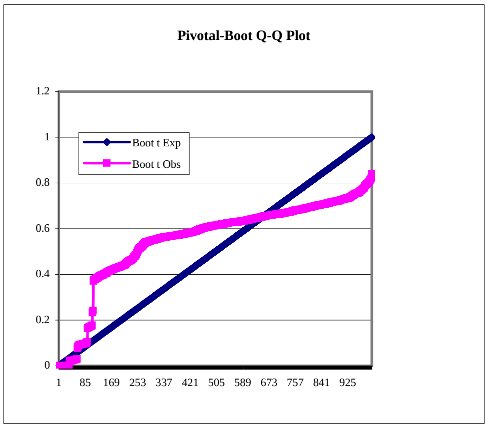
UCL=Upper Confidence Interval

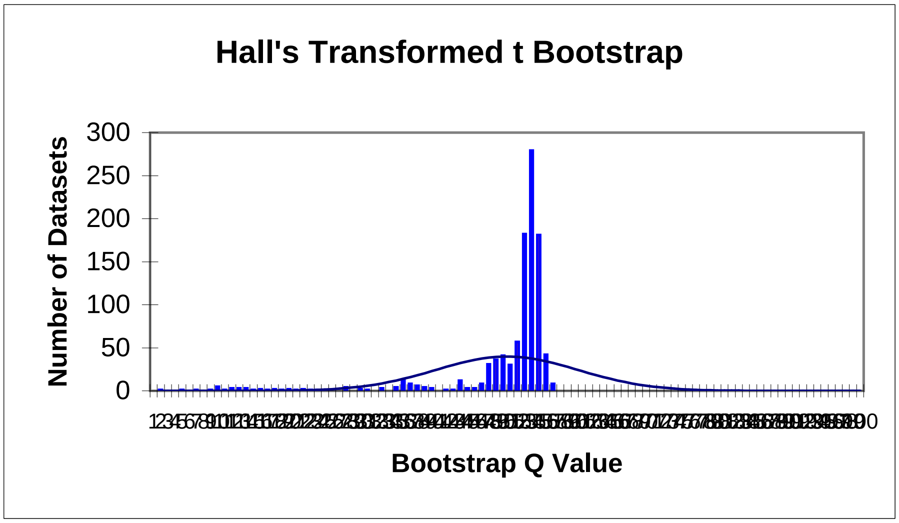
BOOTSTRAP RESULTS FOR OCTANOL-WATER PARTITIONING COEFFCIENTS FOR OCTACHLOROBIPHENYLS OBTAINED FROM EISLER AND BELISLE (1996)

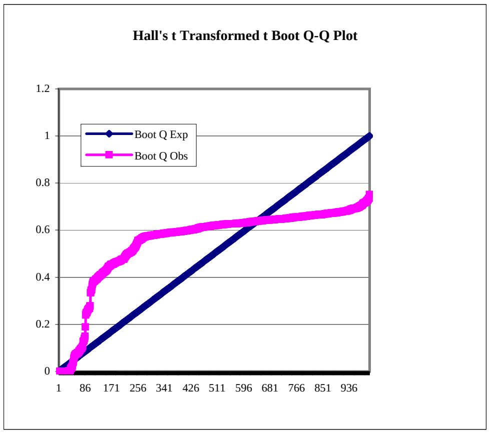












SOLUBILITY, K_{oc}, AND K_{ow} OF SEVERAL PCBs

Compound	Solubility (ppb)	log S	K_{oc}	log K_{oc}
Monochlorobiphenyls				
2-	5,900	3.77	2,951	3.47
3-	3,500	3.54	4,168	3.62
4-	1,190	3.08	7,943	3.90
Dichlorobiphenyls				
2,4-	1,400	3.15	7,244	3.86
2,2'-	1,500	3.18	6,918	3.84
2,4'-	1,260	3.10	8,000	3.90
4,4'-	80	1.90	42,658	4.63
Trichlorobiphenyls				
2,4,4'-	85	1.93	40,738	4.61
2',3,4-	78	1.89	43,652	4.64
Tetrachlorobiphenyls				
2,2',5,5'-	36	1.56	47,000	4.67
2,2',3,3'-	34	1.53	72,443	4.86
2,2',3,5'-	170	2.23	26,915	4.43
2,2',4,4'-	66	1.82	47,863	4.68
2,3',4,4'-	58	1.76	52,480	4.72
2,3',4,5'-	41	1.61	64,565	4.81
3,3',4,4'-	180	2.26	25,633	4.41
Pentachlorobiphenyls				
2,2',3,4,5'-	22	1.34	95,324	4.98
2,2',4,5,5'-	31	1.49	76,948	4.89
Hexachlorobiphenyl				
2,4,5,2',4',5'-	0.95	-0.02	1,200,000	6.08

Source = Chou, S.F.J., and R.A. Griffin. 1986. Solubility and soil mobility of polychlorinated biphenyls. Chapter 5 IN PCBs in the Environment. J.S. Waid, Ed., CRC Press, Boca Ratob, FL.

APPENDIX C

CALCULATION OF HOMOLOG-SPECIFIC VAPOR PRESSURES

VAPOR PRESSURE VALUES FROM OBERG (2001)

PCB	Measured (mm Hg)	Homolog Group	Geomean for Homolog Group (mm Hg)	Vapor Pressure (Pa)
1	1.38E-03	Mono	4.74E-03	6.32E-01
2	7.35E-03			
3	1.05E-02			
4	2.75E-03			
5	m			
6	m			
7	1.38E-03			
8	2.09E-03			
9	1.38E-03			
10	m			
11	6.49E-04			
12	m			
13	m			
14	m			
15	5.35E-04			
16	m			
17	m			
18	1.05E-03			
19	m			
20	m			
21	m			
22	m			
23	m			
24	m			
25	m			
26	m			
27	m			
28	1.95E-04			
29	9.75E-04			
30	7.16E-04			
31	4.00E-04			
32	m			
33	1.03E-04			
34	m			
35	m			
36	m			
37	m			
38	m			
39	m			
40	7.35E-05			
41	m			
42	m			
43	m			
44	m			
45	m			
46	m			
47	8.63E-05			
48	m			
49	8.48E-06			
50	m			
51	m			
52	m			
53	2.25E-05			

VAPOR PRESSURE VALUES FROM OBERG (2001)

PCB	Measured (mm Hg)	Homolog Group	Geomean for Homolog Group (mm Hg)	Vapor Pressure (Pa)
54	m			
55	m			
56	m			
57	m			
58	m			
59	m			
60	m			
61	3.75E-05			
62	m			
63	m			
64	m			
65	m			
66	4.62E-05			
67	m			
68	m			
69	m			
70	4.08E-05			
71	m			
72	m			
73	m			
74	m			
75	m			
76	m			
77	1.64E-05			
78	m			
79	m			
80	m			
81	m			
82	m			
83	m			
84	m			
85	m			
86	6.97E-05			
87	1.70E-05			
88	m			
89	m			
90	m			
91	m			
92	m			
93	m			
94	m			
95	m			
96	m			
97	m			
98	m			
99	2.20E-05			
100	m			
101	2.52E-05			
102	m			
103	m			
104	m			
105	6.53E-06			
106	m			

VAPOR PRESSURE VALUES FROM OBERG (2001)

PCB	Measured (mm Hg)	Homolog Group	Geomean for Homolog Group (mm Hg)	Vapor Pressure (Pa)
107	m			
108	m			
109	m			
110	m			
111	m			
112	m			
113	m			
114	m			
115	m			
116	m			
117	m			
118	8.97E-06			
119	m			
120	m			
121	m			
122	m			
123	m			
124	m			
125	m			
126	m			
127	m			
128	2.56E-06			
129	m			
130	m			
131	m			
132	m			
133	m			
134	1.09E-06			
135	m			
136	m			
137	m			
138	3.79E-06			
139	m			
140	m			
141	m			
142	m			
143	m			
144	m			
145	m			
146	m			
147	m			
148	m			
149	8.43E-06			
150	m			
151	2.29E-06			
152	m			
153	3.43E-06			
154	m			
155	1.20E-05			
156	1.61E-06			
157	m			
158	m			
159	m			

VAPOR PRESSURE VALUES FROM OBERG (2001)

PCB	Measured (mm Hg)	Homolog Group	Geomean for Homolog Group (mm Hg)	Vapor Pressure (Pa)
160	m			
161	m			
162	m			
163	m			
164	m			
165	m			
166	m			
167	m			
168	m			
169	m			
170	6.28E-07			
171	1.40E-06			
172	m			
173	m			
174	m			
175	m			
176	m			
177	m			
178	m	Hepta	1.92E-06	2.56E-04
179	m			
180	9.77E-07			
181	m			
182	m			
183	m			
184	m			
185	m			
186	m			
187	m			
188	m			
189	m			
190	m			
191	m			
192	m			
193	m			
194	m			
195	m	Octa	6.48E-07	8.65E-05
196	m			
197	m			
198	m			
199	m			
200	m			
201	m			
202	3.93E-06			
203	m			
204	m			
205	m			
206	m	Nona	2.07E-07	2.77E-05
207	m			
208	m			
209	1.06E-07	Deca	1.06E-07	1.41E-05

PCB VAPOR PRESSURES OBTAINED FROM THE SCIENTIFIC LITERATURE

Dichlorobiphenyls						
4	0.1844115	1.52E-01	0.4235385	0.33538575		
7	0.18137175	0.17529225	0.21176925			
9	0.1965705	0.23203425				
11	0.033538575	0.06464535	9.22E-02			
12	0.00073562	0.053195625	0.078526875			
15	0.00328293	0.050763825	7.50E-02			
Trichlorobiphenylas						
18	0.0761964	3.55E-02	0.0903819	0.076703025		
26	0.032322675	1.82E-02	0.0352611	0.041239275		
28	0.014489475	1.52E-02	0.027661725	0.033538575		
30	0.0644427	0.09463755	0.11044425			
Tetrachlorobiphenyls						
40	0.00109431	4.56E-03	1.11E-02	0.008805143		
52	0.0129696	9.02E-02	1.93E-02	0.01844115		
53	0.006707715	1.11E-02	0.035565075	0.026648475		
54	0.00226968	6.59E-02	0.056640675			
77	1.82E-05	0.001398285	0.002117693		5.87E-05	
Pentachlorobiphenyls						
101	5.27E-04	1.42E-03	0.003576773	0.003586905		
104	0.00433671	0.00433671				
Hexachlorobiphenyls						
128	2.94E-06	9.82853E-05	0.000358691	0.000366797		
138					5.33E-04	
153	3.24E-05	2.53E-04	0.006626655	0.007001558	5.07E-05	1.20E-04
155	0.000480281	0.004427903				
169					5.36E-05	

First four columns are from Fielder (2001) and the last two are from ATSDR (1995)
All vapor pressures are in Pascals (Pa)

STATISTICAL ANALYSIS OF VAPOR PRESSURES OBTAINED FROM THE SCIENTIFIC LITERATURE

Dichlorobiphenyl

The data are best described as normally distributed and there were a sufficient number of values to perform a statistical analysis.

Vapor presure is in Pascals (Pa)

	Value
1	0.1844115
2	0.1813718
3	0.1965705
4	0.0335386
5	0.0007356
6	0.0032829
7	0.1519875
8	0.1752923
9	0.2320343
10	0.0646454
11	0.0531956
12	0.0507638
13	0.4235385
14	0.2117693
15	0.0922058
16	0.0785269
17	0.0749805
18	0.3353858

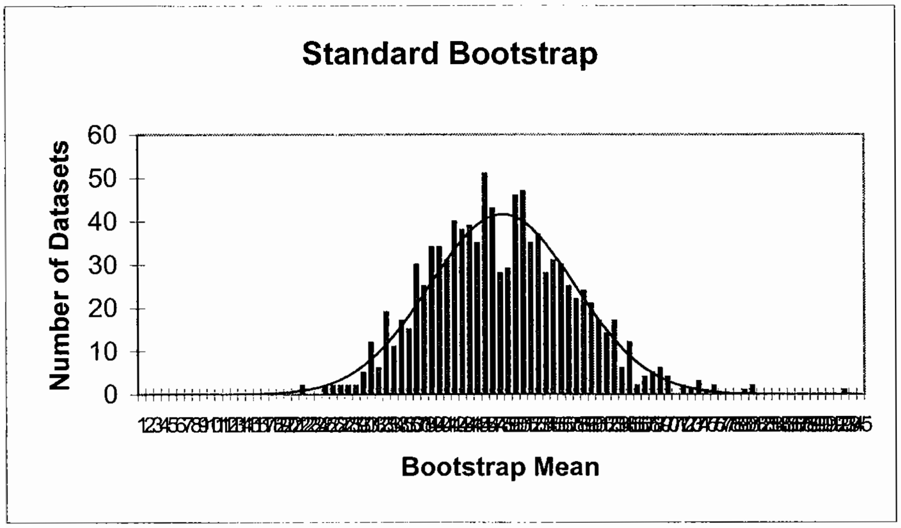
Recommended Mean	Normal Mean	1
Recommended UCL	UCL based on t-statistic	0.188130706

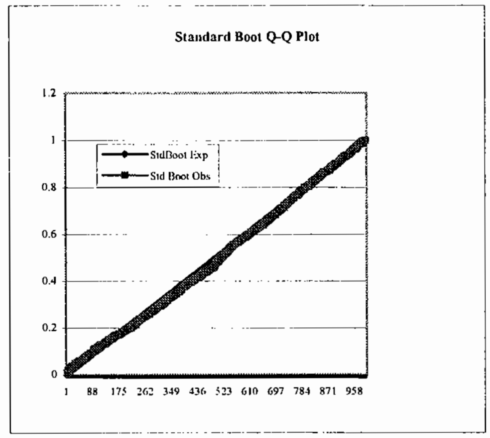
Raw Data Results					
Number of Values		18			
Maximum Value		4.24E-01	Minimum Value		7.36E-04
Normal (Non-transformed) Results					
Normal Mean		1.41E-01	Mean Standard Error		2.69E-02
Standard Deviation		1.14E-01	Coefficient of Variance (%)		81%
Dataset Skewness	Pass	8.24E-01	Dataset Kurtosis	Pass	2.94E+00
Tested for Normality		W-Test	NormalityResult (a = 0.05)		Pass
Critical Value		8.97E-01	Calculated Value for dataset		9.14E-01
90% UCL using t-statistic		1.77E-01	95% UCL using -t-statistic		1.88E-01
Natural Log-Transformed Results					
MVUE of the log-mean		2.41E-01	Standard error of the log-me		1.08E-01
Standard Deviation		1.60E+00	Coefficient of Variance (%)		-62%
Dataset Skewness	Fail	-1.6E+00	Dataset Kurtosis	Pass	4.98E+00
Tested for Normality		W-Test	Normality Result (a = 0.05)		Fail
Critical Value		8.97E-01	Calculated Value for dataset		7.87E-01
Anderson Darling (AD) A^2		1.39E+00	AD Probability	Fail	2.06E-01
90% UCL of the MVUE		7.59E-01	95% UCL of the MVUE		1.12E+00
Jackknife Results					
Jackknifed Mean		1.41E-01	Jackknifed Standard Error		2.69E-02
90% UCL of the mean		1.77E-01	95% UCL of the mean		1.88E-01
90% UCL of the MVUE[2]		3.68E-01	95% UCL of the MVUE[2]		4.01E-01

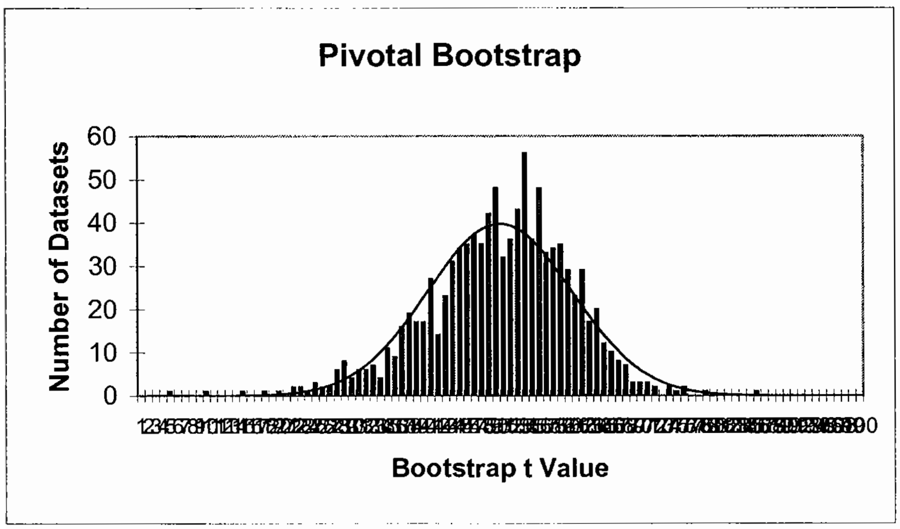
Bootstrap Results (Raw Data)						
Standard Bootstrap	Mean	1.40E-01	90% UCL	1.75E-01	95% UCL	1.84E-01
Skewness	3.52E-01		Kurtosis	3.41E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Pivitol (t) Bootstrap	90% UCL	1.88E-01	95% UCL		2.03E-01	
Skewness	-5.96E-01		Kurtosis	4.46E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Hall's t Bootstrap	90% UCL	1.83E-01	95% UCL		1.97E-01	
Skewness	-1.5E+00		Kurtosis	9.86E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						

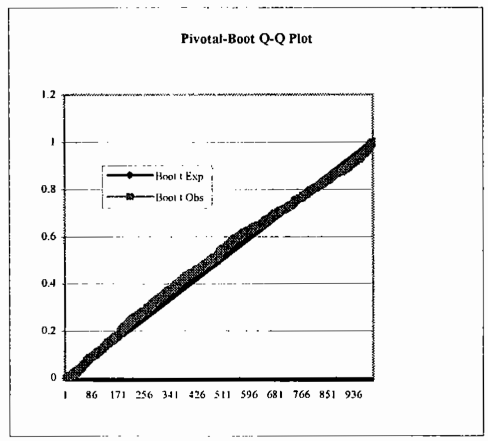
2 = Using the Jackknife
MVUE=Minimum Variance Unbiased Estimator
UCL=Upper Confidence Interval

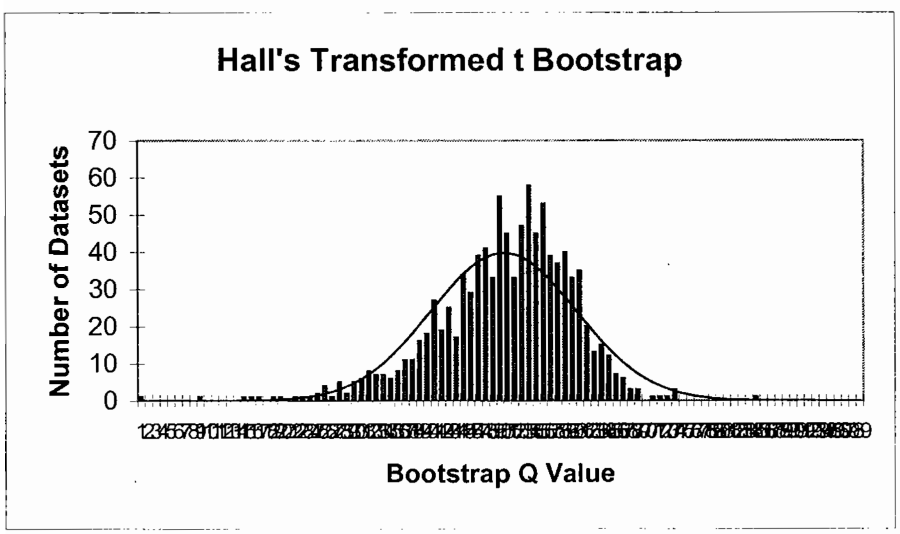
BOOTSTRAP RESULTS FOR VAPOR PRESSURES FOR DICHLOROBIPHENYLS OBTAINED FROM THE SCIENTIFIC LITERATURE

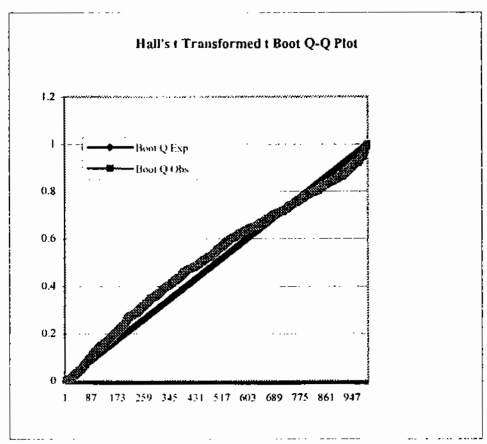












STATISTICAL ANALYSIS OF VAPOR PRESSURES OBTAINED FROM THE SCIENTIFIC LITERATURE

Trichlorobiphenyl

The data are best described as normally distributed and there were a sufficient number of detected values to perform a statistical analysis. Use the normal mean and t-statistic derived UCLs as EPCs

Vapor presure is in Pascals (Pa)

	Value
1	0.0761964
2	0.0323227
3	0.0144895
4	0.0644427
5	0.0354638
6	0.0182385
7	0.0151988
8	0.0946376
9	0.0903819
10	0.0352611
11	0.0276617
12	0.1104443
13	0.076703
14	0.0412393
15	0.0335386

Recommended Mean	Normal Mean	1
Recommended UCL	UCL based on t-statistic	0.065429299

Raw Data Results					
Number of Values		15			
Maximum Value		1.10E-01	Minimum Value		1.45E-02
Normal (Non-transformed) Results					
Normal Mean		5.11E-02	Mean Standard Error		8.15E-03
Standard Deviation		3.16E-02	Coefficient of Variance (%)		62%
Dataset Skewness	Pass	4.74E-01	Dataset Kurtosis	Fail	1.65E+00
Tested for Normality		W-Test	NormalityResult (a = 0.05)		Pass
Critical Value		8.81E-01	Calculated Value for dataset		8.97E-01
90% UCL using t-statistic		6.20E-02	95% UCL using -t-statistic		6.54E-02
Natural Log-Transformed Results					
MVUE of the log-mean		5.16E-02	Standard error of the log-me		9.39E-03
Standard Deviation		6.71E-01	Coefficient of Variance (%)		-21%
Dataset Skewness	Pass	-1.19E-01	Dataset Kurtosis	Fail	1.59E+00
Tested for Normality		W-Test	Normality Result (a = 0.05)		Pass
Critical Value		8.81E-01	Calculated Value for dataset		9.31E-01
Anderson Darling (AD) A^2		3.92E-01	AD Probability	Pass	8.58E-01
90% UCL of the MVUE		7.08E-02	95% UCL of the MVUE		7.89E-02
Jackknife Results					
Jackknifed Mean		5.11E-02	Jackknifed Standard Error		8.15E-03
90% UCL of the mean		6.20E-02	95% UCL of the mean		6.54E-02
90% UCL of the MVUE[2]		6.36E-02	95% UCL of the MVUE[2]		6.73E-02

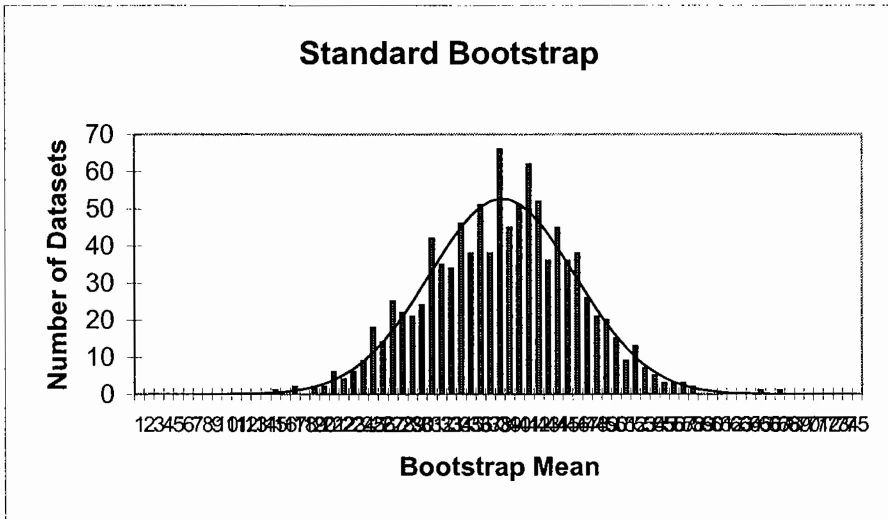
Bootstrap Results (Raw Data)						
Standard Bootstrap	Mean	5.13E-02	90% UCL	6.12E-02	95% UCL	6.41E-02
Skewness	-9.45E-03		Kurtosis	2.96E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Pivitol (t) Bootstrap	90% UCL	6.38E-02	95% UCL	6.77E-02		
Skewness	-7.97E-01		Kurtosis	5.64E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Hall's t Bootstrap	90% UCL	6.38E-02	95% UCL	6.71E-02		
Skewness	-1.9E+00		Kurtosis	1.36E+01		
Quantile fit is good - Bootstrap Output is Normal or nearly so						

2 = Using the Jackknife

MVUE=Minimum Variance Unbiased Estimator

UCL=Upper Confidence Interval

BOOTSTRAP RESULTS FOR VAPOR PRESSURES FOR TRICHLOROBIPHENYLS OBTAINED FROM THE SCIENTIFIC LITERATURE



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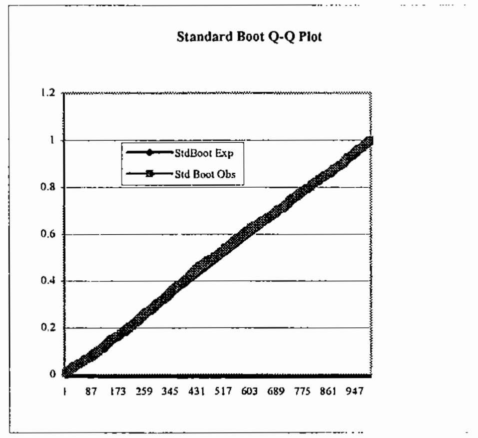
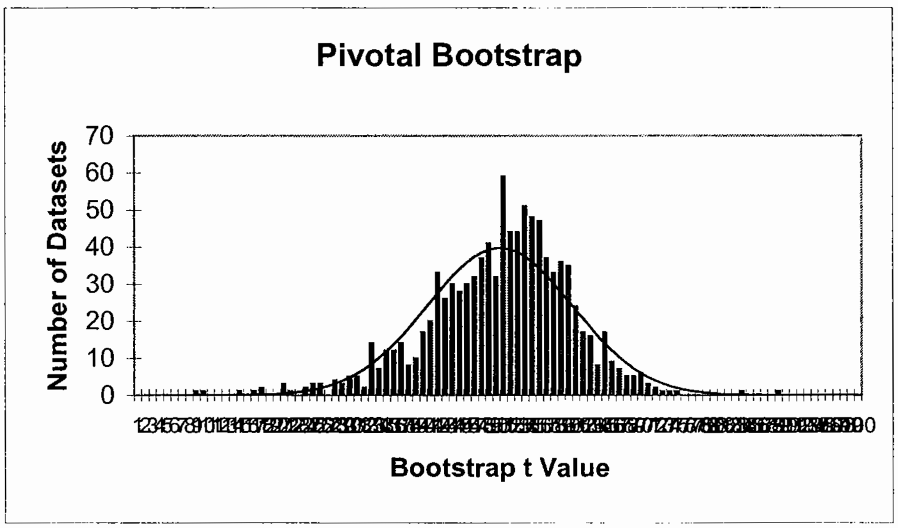
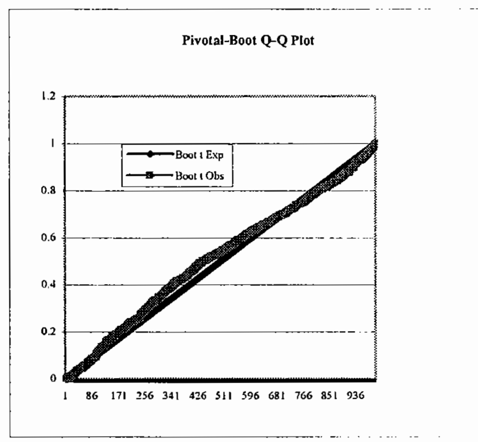
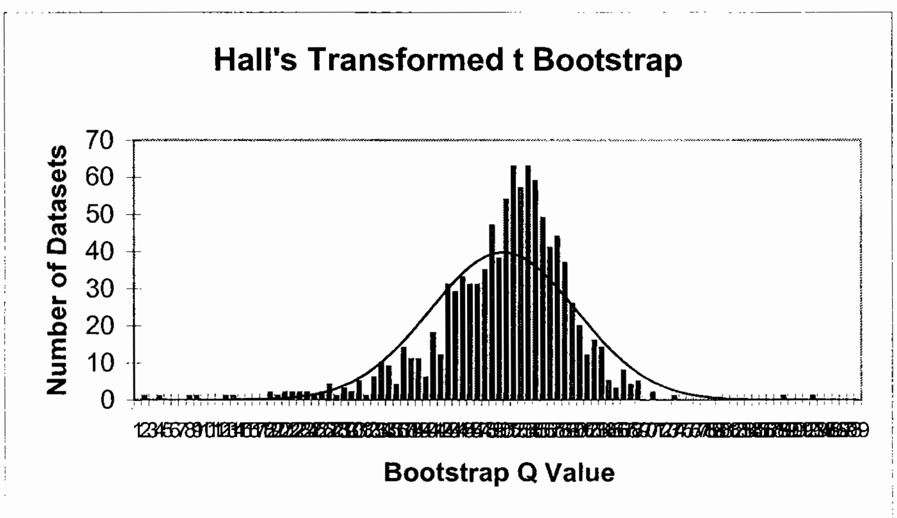
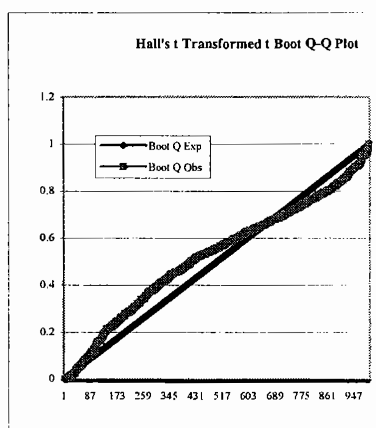










STATISTICAL ANALYSIS OF VAPOR PRESSURES OBTAINED FROM THE SCIENTIFIC LITERATURE

Tetrachlorobiphenyl

There is a sufficient number of values for statistical analysis - the data were found to be non-normal with high skewness, however, the Hall's transformed t bootstrap failed to normalize the dataset

Vapor presure is in Pascals (Pa)

	Value
1	0.0010943
2	0.0129696
3	0.0067077
4	0.0022697
5	1.824E-05
6	0.0045596
7	0.0901793
8	0.0111458
9	0.0658613
10	0.0013983
11	0.0111458
12	0.0192518
13	0.0355651
14	0.0566407
15	0.0021177
16	0.0088051
17	0.0184412
18	0.0266485

Recommended Mean	Bootstrap Mean	1
Recommended UCL	Standard Bootstrap UCL	0.030500704

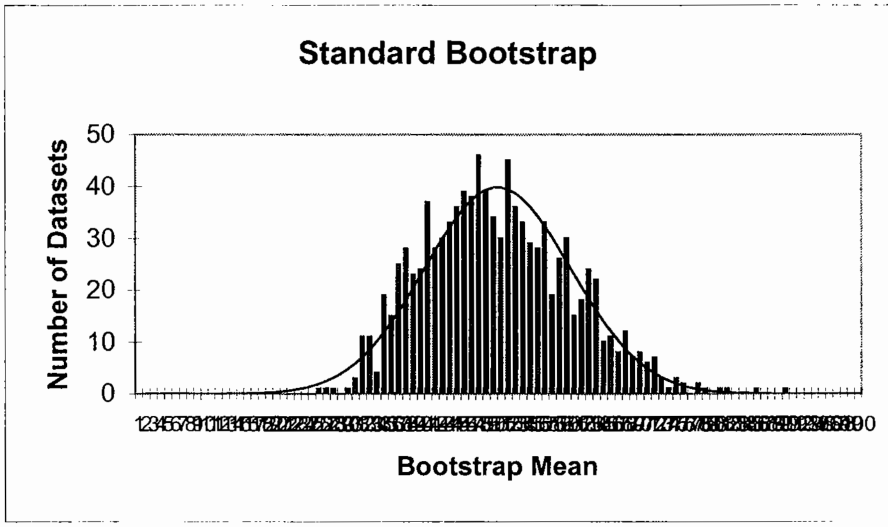
Raw Data Results					
Number of Values	18				
Maximum Value	9.02E-02		Minimum Value		1.82E-05
Normal (Non-transformed) Results					
Normal Mean	2.08E-02		Mean Standard Error		6.03E-03
Standard Deviation	2.56E-02		Coefficient of Variance (%)		123%
Dataset Skewness	Fail	1.41E+00	Dataset Kurtosis	Pass	3.86E+00
Tested for Normality	W-Test		NormalityResult (a = 0.05)		Fail
Critical Value	8.97E-01		Calculated Value for dataset		7.74E-01
90% UCL using t-statistic	2.89E-02		95% UCL using -t-statistic		3.13E-02
Natural Log-Transformed Results					
MVUE of the log-mean	4.23E-02		Standard error of the log-me		2.39E-02
Standard Deviation	1.99E+00		Coefficient of Variance (%)		-41%
Dataset Skewness	Fail	-1.4E+00	Dataset Kurtosis	Pass	5.06E+00
Tested for Normality	W-Test		Normality Result (a = 0.05)		Fail
Critical Value	8.97E-01		Calculated Value for dataset		8.73E-01
Anderson Darling (AD) A^2	6.10E-01		AD Probability	Pass	6.37E-01
90% UCL of the MVUE	2.44E-01		95% UCL of the MVUE		4.36E-01
Jackknife Results					
Jackknifed Mean	2.08E-02		Jackknifed Standard Error		6.03E-03
90% UCL of the mean	2.89E-02		95% UCL of the mean		3.13E-02
90% UCL of the MVUE[2]	7.69E-02		95% UCL of the MVUE[2]		8.69E-02

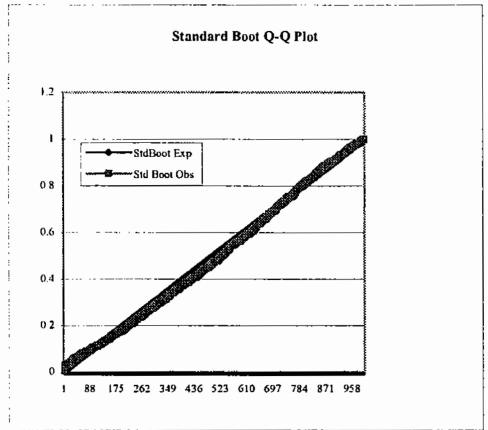
Bootstrap Results (Raw Data)						
Standard Bootstrap	Mean	2.08E-02	90% UCL	2.84E-02	95% UCL	3.05E-02
Skewness	3.78E-01		Kurtosis	2.92E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Pivitol (t) Bootstrap	90% UCL	3.27E-02	95% UCL		3.73E-02	
Skewness	-2.0E+00		Kurtosis	1.33E+01		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Hall's t Bootstrap	90% UCL	3.37E-02	95% UCL		3.57E-02	
Skewness	-3.4E+00		Kurtosis	2.53E+01		
Quantile fit is poor do not use Bootstrap Results						

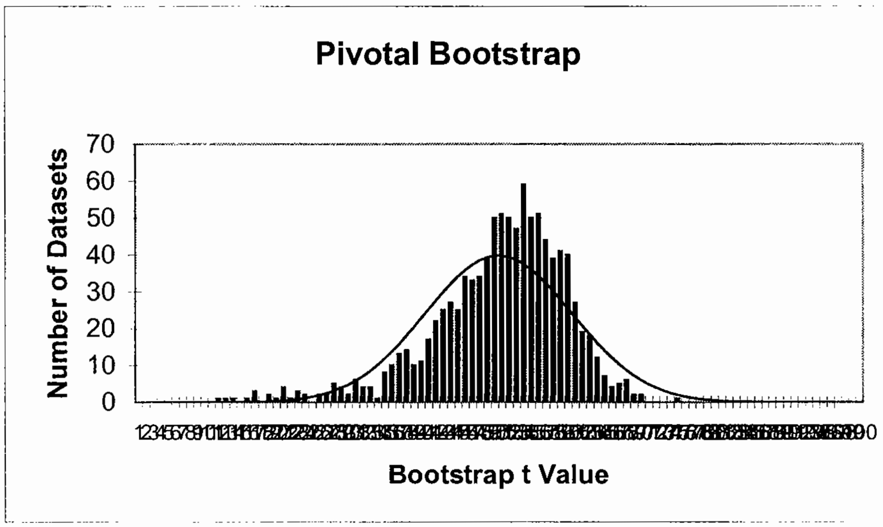
2 = Using the Jackknife
MVUE=Minimum Variance Unbiased Estimator
UCL=Upper Confidence Interval

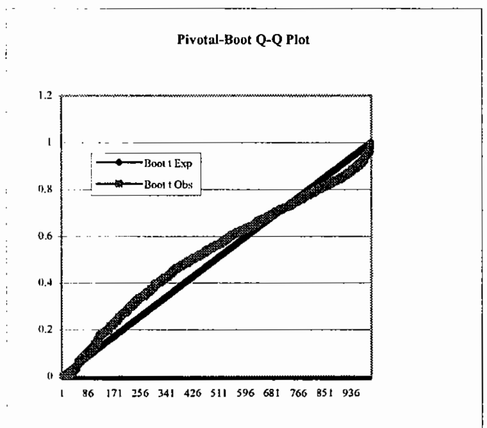
BOOTSTRAP RESULTS FOR VAPOR PRESSURES FOR TETRACHLOROBIPHENYLS OBTAINED FROM THE SCIENTIFIC LITERATURE (Including suspected outlier)

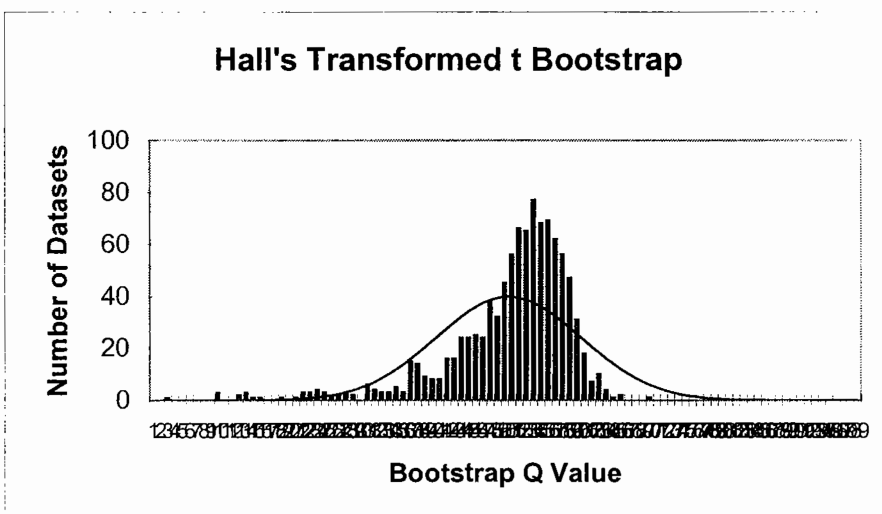
1

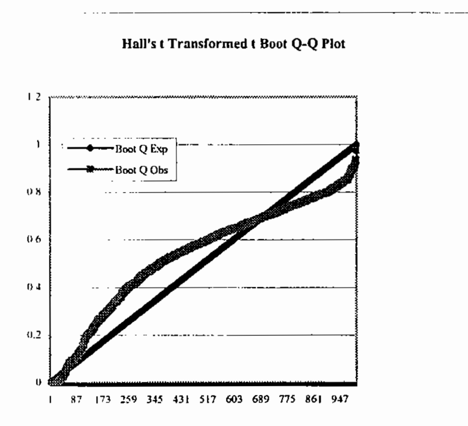












STATISTICAL ANALYSIS OF VAPOR PRESSURES OBTAINED FROM THE SCIENTIFIC LITERATURE

Pentachlorobiphenyl

The data are best described as normally distributed and there were a sufficient number of detected values to perform a statistical analysis.

Vapor presure is in Pascals (Pa)

	Value
1	0.0005269
2	0.0043367
3	0.0014186
4	0.0043367
5	0.0035768
6	0.0035869

Recommended Mean	Normal Mean	1
Recommended UCL	UCL based on t-statistic	0.004283067

Raw Data Results					
Number of Values	6				
Maximum Value	4.34E-03		Minimum Value		5.27E-04
Normal (Non-transformed) Results					
Normal Mean	2.96E-03		Mean Standard Error		6.55E-04
Standard Deviation	1.60E-03		Coefficient of Variance (%)		54%
Dataset Skewness	Pass	-5.06E-01	Dataset Kurtosis	Fail	1.22E+00
Tested for Normality	W-Test		NormalityResult (a = 0.05)		Pass
Critical Value	7.88E-01		Calculated Value for dataset		8.31E-01
90% UCL using t-statistic	3.93E-03		95% UCL using -t-statistic		4.28E-03
Natural Log-Transformed Results					
MVUE of the log-mean	3.17E-03		Standard error of the log-me		1.09E-03
Standard Deviation	8.48E-01		Coefficient of Variance (%)		-14%
Dataset Skewness	Pass	-8.16E-01	Dataset Kurtosis	Pass	1.79E+00
Tested for Normality	W-Test		Normality Result (a = 0.05)		Fail
Critical Value	7.88E-01		Calculated Value for dataset		7.75E-01
Anderson Darling (AD) A^2	6.77E-01		AD Probability	Pass	5.78E-01
90% UCL of the MVUE	7.99E-03		95% UCL of the MVUE		1.20E-02
Jackknife Results					
Jackknifed Mean	2.96E-03		Jackknifed Standard Error		6.55E-04
90% UCL of the mean	3.93E-03		95% UCL of the mean		4.28E-03
90% UCL of the MVUE[2]	4.31E-03		95% UCL of the MVUE[2]		4.67E-03

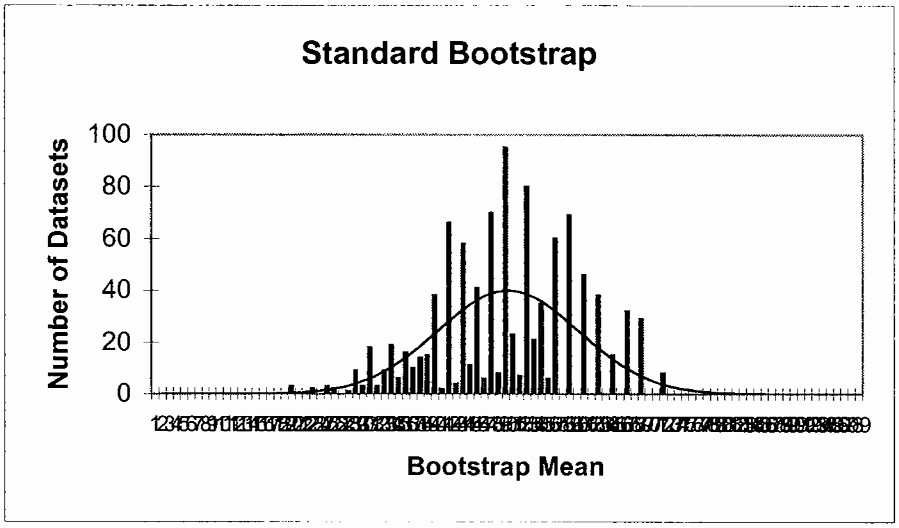
Bootstrap Results (Raw Data)						
Standard Bootstrap	Mean	2.96E-03	90% UCL	3.71E-03	95% UCL	3.92E-03
Skewness	-1.45E-01		Kurtosis	2.71E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so						
Pivitol (t) Bootstrap	90% UCL	3.83E-03	95% UCL	4.05E-03		
Skewness	2.13E+01		Kurtosis	4.68E+02		
Quantile fit is poor do not use Bootstrap Results						
Hall's t Bootstrap	90% UCL	3.73E-03	95% UCL	4.05E-03		
Skewness	1.69E+01		Kurtosis	3.29E+02		
Quantile fit is poor do not use Bootstrap Results						

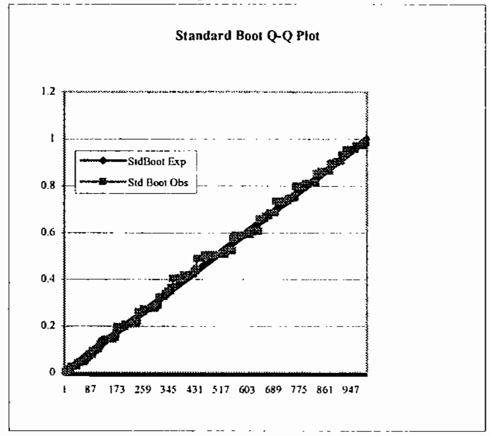
2 = Using the Jackknife

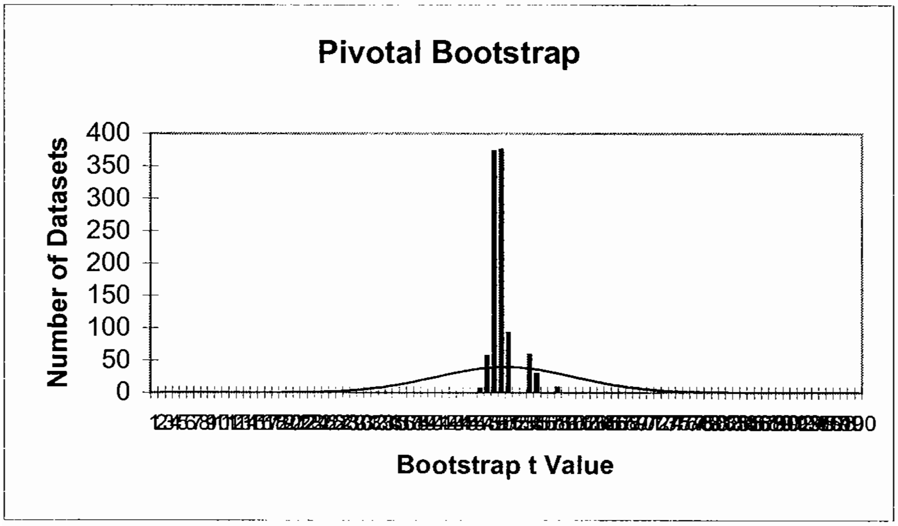
MVUE=Minimum Variance Unbiased Estimator

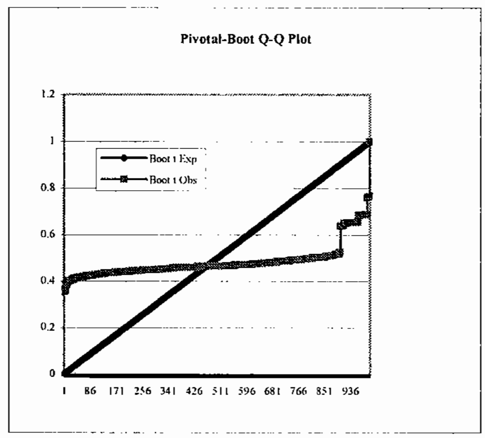
UCL=Upper Confidence Interval

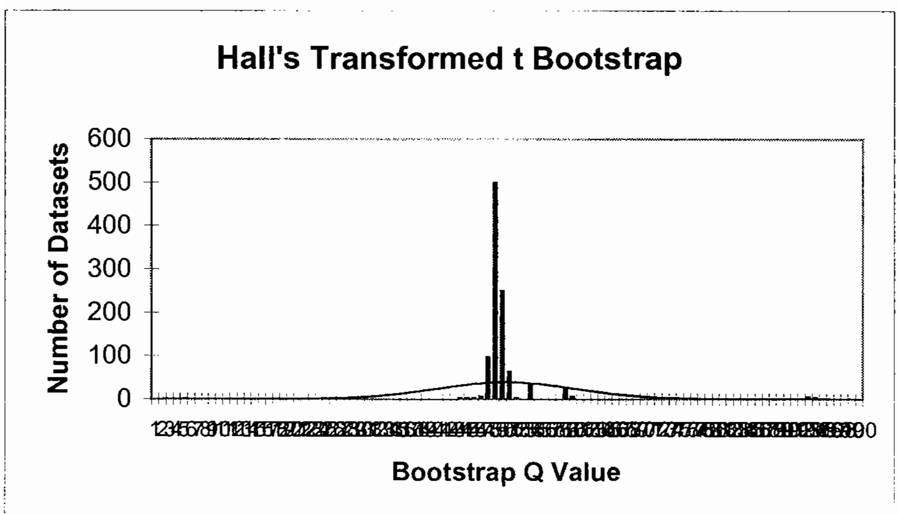
BOOTSTRAP RESULTS FOR VAPOR PRESSURES FOR PENTACHLOROBIPHENYLS OBTAINED FROM THE SCIENTIFIC LITERATURE

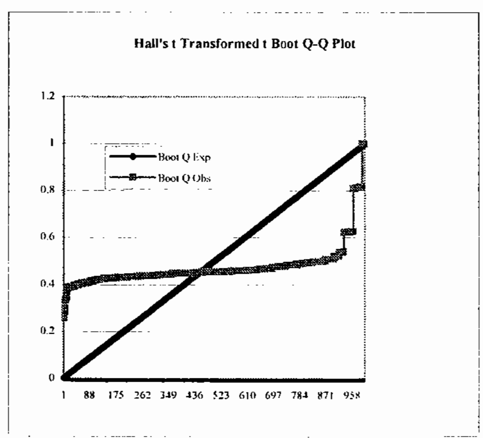












STATISTICAL ANALYSIS OF VAPOR PRESSURES OBTAINED FROM THE SCIENTIFIC LITERATURE

Hexachlorobiphenyl

The data are best described as log-normally distributed and there were a sufficient number of detected values to perform statistical analysis. The CV is > 100%

Vapor presure is in Pascals (Pa)

	Value
1	2.938E-06
2	3.242E-05
3	0.0004803
4	9.829E-05
5	0.0002533
6	0.0044279
7	0.0003587
8	0.0066267
9	0.0003668
10	0.0070016

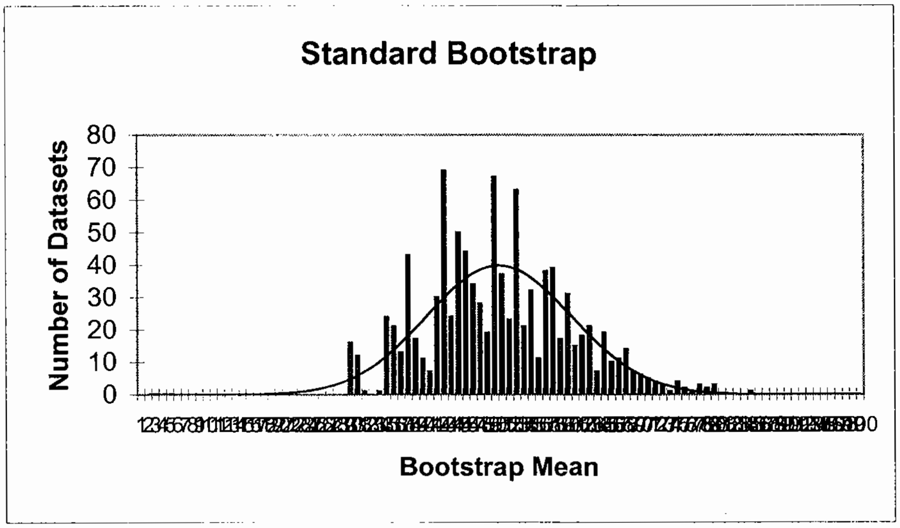
Recommended Mean	MVUE of the log-mean	1
Recommended UCL	UCL based on Jackknifed MVUE	0.009196063

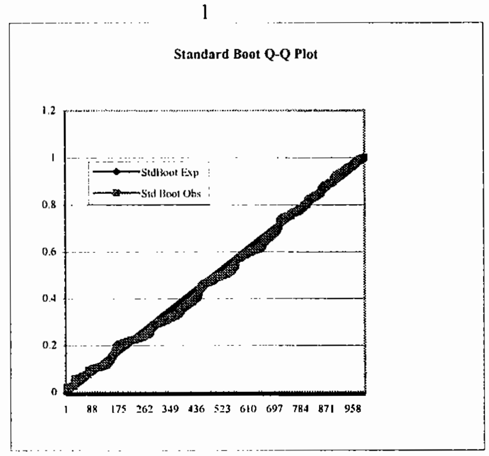
Raw Data Results					
Number of Values		10			
Maximum Value		7.00E-03	Minimum Value		2.94E-06
Normal (Non-transformed) Results					
Normal Mean		1.96E-03	Mean Standard Error		9.10E-04
Standard Deviation		2.88E-03	Coefficient of Variance (%)		146%
Dataset Skewness	Pass	8.66E-01	Dataset Kurtosis	Pass	1.78E+00
Tested for Normality		W-Test	NormalityResult (a = 0.05)		Fail
Critical Value		8.42E-01	Calculated Value for dataset		6.85E-01
90% UCL using t-statistic		3.22E-03	95% UCL using -t-statistic		3.63E-03
Natural Log-Transformed Results					
MVUE of the log-mean		3.43E-03	Standard error of the log-me		2.61E-03
Standard Deviation		2.46E+00	Coefficient of Variance (%)		-31%
Dataset Skewness	Pass	-3.89E-01	Dataset Kurtosis	Pass	2.07E+00
Tested for Normality		W-Test	Normality Result (a = 0.05)		Pass
Critical Value		8.42E-01	Calculated Value for dataset		9.29E-01
Anderson Darling (AD) A^2		3.31E-01	AD Probability	Pass	9.14E-01
90% UCL of the MVUE		2.78E-01	95% UCL of the MVUE		1.52E+00
Jackknife Results					
Jackknifed Mean		1.96E-03	Jackknifed Standard Error		9.10E-04
90% UCL of the mean		3.22E-03	95% UCL of the mean		3.63E-03
90% UCL of the MVUE^2		7.89E-03	95% UCL of the MVUE^2		9.20E-03

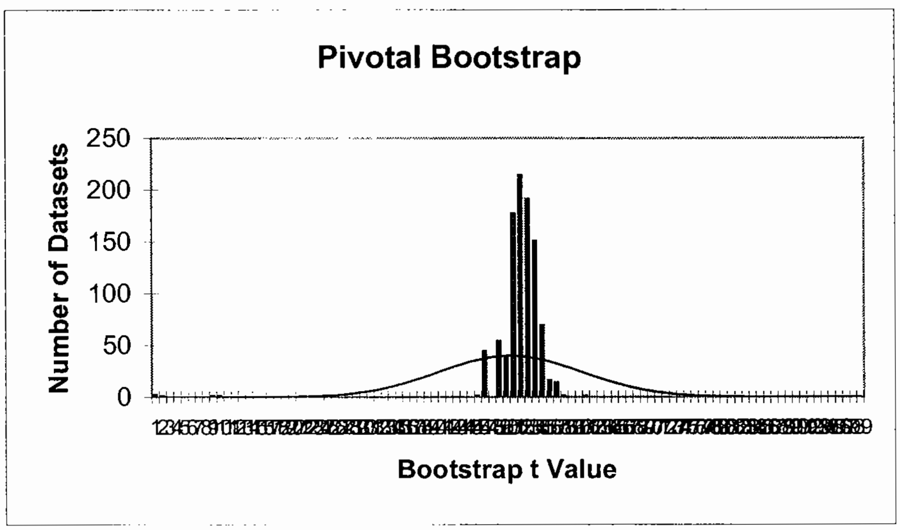
Bootstrap Results (Raw Data)							
Standard Bootstrap		Mean	1.99E-03	90% UCL	3.12E-03	95% UCL	3.44E-03
	Skewness	3.30E-01		Kurtosis	2.89E+00		
Quantile fit is good - Bootstrap Output is Normal or nearly so							
Pivitol (t) Bootstrap		90% UCL	3.56E-03		95% UCL		4.98E-03
	Skewness	-5.4E+00		Kurtosis	3.16E+01		
Quantile fit is poor do not use Bootstrap Results							
Hall's t Bootstrap		90% UCL	3.55E-03		95% UCL		4.97E-03
	Skewness	-1.0E+01		Kurtosis	1.28E+02		
Quantile fit is poor do not use Bootstrap Results							

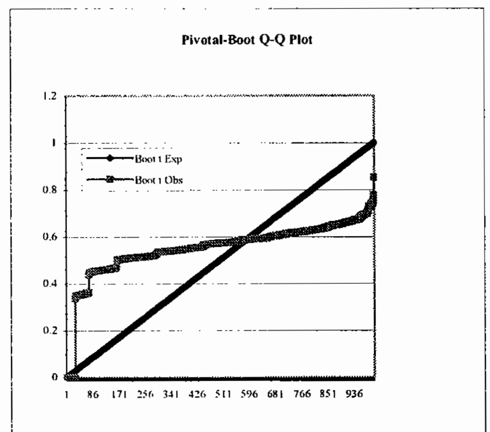
2 = Using the Jackknife
MVUE=Minimum Variance Unbiased Estimator
UCL=Upper Confidence Interval

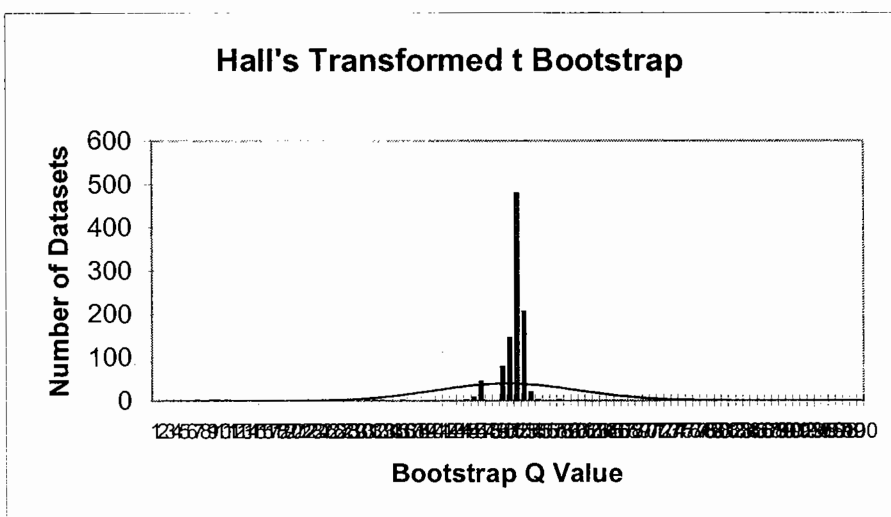
BOOTSTRAP RESULTS FOR VAPOR PRESSURES FOR HEXACHLOROBIPHENYLS OBTAINED FROM THE SCIENTIFIC LITERATURE

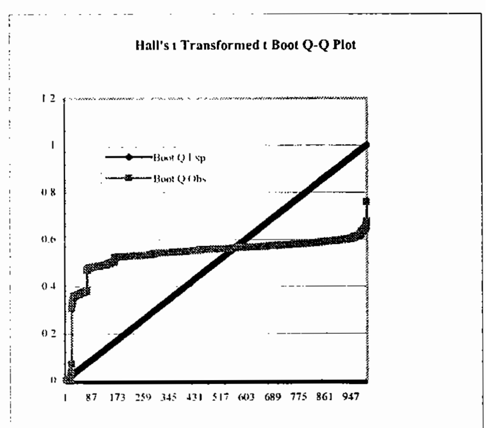












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Prediction of physical properties for PCB congeners from molecular descriptors

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Keywords: Polychlorinated biphenyls, QSPR, principal components regression, PLS modeling.

Abstract

A methodology is described to model quantitative structure-property relationships that can accept significant contamination with "bad data". This approach is used to model and predict the vapor pressures, the water solubilities, the octanol-water partitioning coefficients and the Henry's laws coefficients for all 209 congeners of polychlorinated biphenyls (PCB). The model predictions seem to provide a reliable summary and extension of the currently available database on these compounds.

Introduction

The physical properties for organic chemical compounds are important in determining their distribution and fate in the environment[1]. Examples of such properties are the vapor pressure, the water solubility, the octanol-water partition coefficient and the Henry's law coefficient. Experimental measurements of these properties have become easier with the introduction of new methods, e.g. determination of octanol-water partitioning using gas chromatography, but the number of compounds under consideration still makes it necessary to also use models for estimation.

Polychlorinated biphenyls (PCB) are a group of 209 different congeners that have attracted much attention as environmental pollutants. On May 22 2001, 127 governments adopted the

Stockholm Convention on Persistent Organic Pollutants. PCBs were among the chemicals initially selected for elimination from production and use[2]. Production of PCB has been banned in the industrialized world since many years, but large quantities still remain in the environment[3]. It is therefore still of utmost importance to estimate and monitor their fate in the environment and the biological food chains. The physical properties of the PCBs can also be used as input in calculating relationships to biological activity[4], or to other physical properties[5]. Measured physical properties have been reported for 20-60% of the PCB congeners[6].

The molecular structure holds the key to predicting the physical properties, and it is easy to recognize the trends within a homologous group such as the PCBs[7,8]. The literature contains many estimation methods, and well known are the additive group and bond contribution methods[9,10,11,12,13,14]. These methods are fairly robust and can be applied to a wide variety of organic molecules. A robust and general method will however by definition lack some accuracy and precision when considering local phenomena, such as the properties within a specific compound group.

Topological, geometrical and electronic descriptors can give more in-depth descriptions of the molecules and serve as a basis for developing predictive models with an improved accuracy and precision[15,16,17]. The purpose of this investigation is to develop multivariate calibration models and predict the vapor pressure, the water solubility, the octanol-water partitioning, and the Henry's law constant for all 209 PCB congeners. We will also explore the possibilities of using these models to validate available experimental data.

Experimental

Experimentally determined values for the physical properties were obtained from the PhysProp Database (Syracuse Research Corporation, Syracuse, NY, USA)[6]. Vapor pressures were reported for 42 congeners, water solubilities for 122 congeners, octanol-water partitioning coefficients for 92 congeners, and Henry's law constants for 91 congeners. The data in the PhysProp Database are collected from a large number of investigators, so we can assume that there is variation both within and between the various laboratories and investigators.

With the purpose of validating the methodology we also have included a set of experimental data with an expected high accuracy and precision in the form of retention times in gas chromatography using different columns and separation conditions. Retention time data were obtained from the manufacturers data sheets[18,19,20].

The chemical structure of each congener was sketched on a PC using the software HyperChem (HyperCube, Inc., Gainesville, Florida, USA). Each compound was modeled using the force-field routine MM+, an extension by HyperCube of the standard MM2 force field[21]. The molecular structures were then used as input for the generation of 853 descriptors with the software Dragon (Milano Chemometrics and QSAR Research Group, University of Milano-Bicocca, Milano, Italy), listed in the enclosed text file varfile.txt. Todeschini and Consonni have reviewed these molecular descriptors[22].

The multivariate analysis and calibration was carried out with the software Unscrambler (CAMO ASA, Oslo, Norway), Matlab (MathWorks, Inc., Natick, MA, USA) and Progress (Rousseeuw & Leroy, 1987). Principal component analysis (PCA), principal component regression (PCR), PLS-regression (PLSR) and least median of squares regression (LMSR) were used as the modeling methods. Martens and Næs have reviewed PCA, PCR and PLSR[23]. Rousseeuw and Leroy have reviewed LMSR and other methods for robust regression and outlier detection[24].

Results and discussion

Here we use the numbering system for PCB congeners currently assigned by Ballschmiter and the International Union of Pure and Applied Chemistry[25].

447 descriptors with constant values for all congeners were excluded from the data analysis. The raw data hence consist of 406 descriptor variables (varlist.txt) and the seven dependent

response variables. The raw data is listed in the enclosed tab separated text file rawdat.txt (the first row lists the column headings, each following row corresponds to a congener and each column to a variable). All descriptor variables were autoscaled to zero mean and unit variance. The three dependent retention-times variables were also autoscaled, while the four dependent physical property variables were log-transformed prior to data analysis and modeling.

The descriptor data were initially modeled using principal component analysis (PCA). A five-component model explained 65% of the variance in the calibration data and 59% of the variance in ten randomly selected cross-validation segments. The first two score vectors are shown in figure 1. All five score vectors are listed in the enclosed tab separated text file scores.txt.

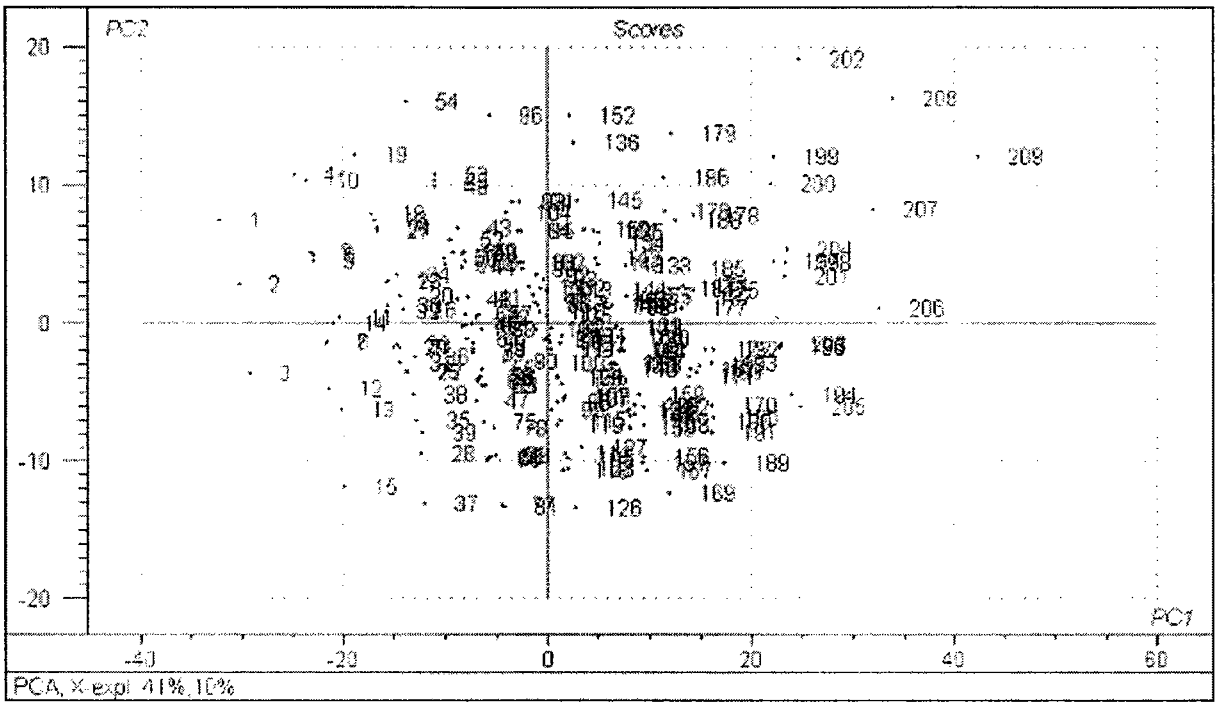

Figure 1
Scores for the two first principal components (IUPAC-numbers shown for each congener).

The position of the congeners on the score plot relates to the chemical structures. The congener groups line up from left to the right with increasing number of chlorine atoms. In a similar manner the vertical distribution reflect the substitution pattern, with non-ortho chlorinated biphenyls ("co-planar") at the bottom and those with tri- and tetra-ortho substitution at the top. The ortho-substitution pattern directly influences the energy barrier of rotation and it is also correlated to the biological activities of these compounds[26].

The first five principal components were used as independent variables for LMSR. Such a semi-robust regression model was estimated for each of the dependent physical property variables and subsequently used to identify outliers in the dependent variables. An object was declared an outlier if the standardized residual was larger than 2.5. PCR and PLSR can also be extended to become robust both with regard to independent and dependent variables[27,28], but this would not serve any purpose in the present investigation.

As a second step, a reweighted PCR could be run by assigning zero weight, or some value on a scale between zero and one, to the outlying objects. Instead we have proceeded with a reweighted PLSR were each outlying object was assigned zero weight, i.e. removed from the computation of the regression model. The PLSR1 procedure was used to obtain models with optimal accuracy and precision. A further step to get parsimonious models was to assign zero weight to descriptor variables with minor influence in the PLS1-regression. These variables were selected on the criteria that the weighted regression coefficients were approximately less than half of the maximum values when all variables were included.

Vapor pressure

Experimental measurements were available for 42 congeners. Outlying objects were identified using the robust PCR procedure described above. 34 objects (objlist1.txt) and 260 descriptor variables (varlist1.txt) were assigned non-zero weight in the successive PLSR1-regression. The calibration model was validated using a test set of 12 randomly selected objects (testset1.txt). The number of latent variables to keep in the PLS-model was estimated to one, yielding a model with a coefficient of determination R^2 for the test set of 0.972. The standard error of prediction SEP, estimated from the test set, was 0.21 (log mm

Hg). Figure 2 show predicted versus measured results for all 42 congeners, with the eight outlying objects marked as filled rectangles.

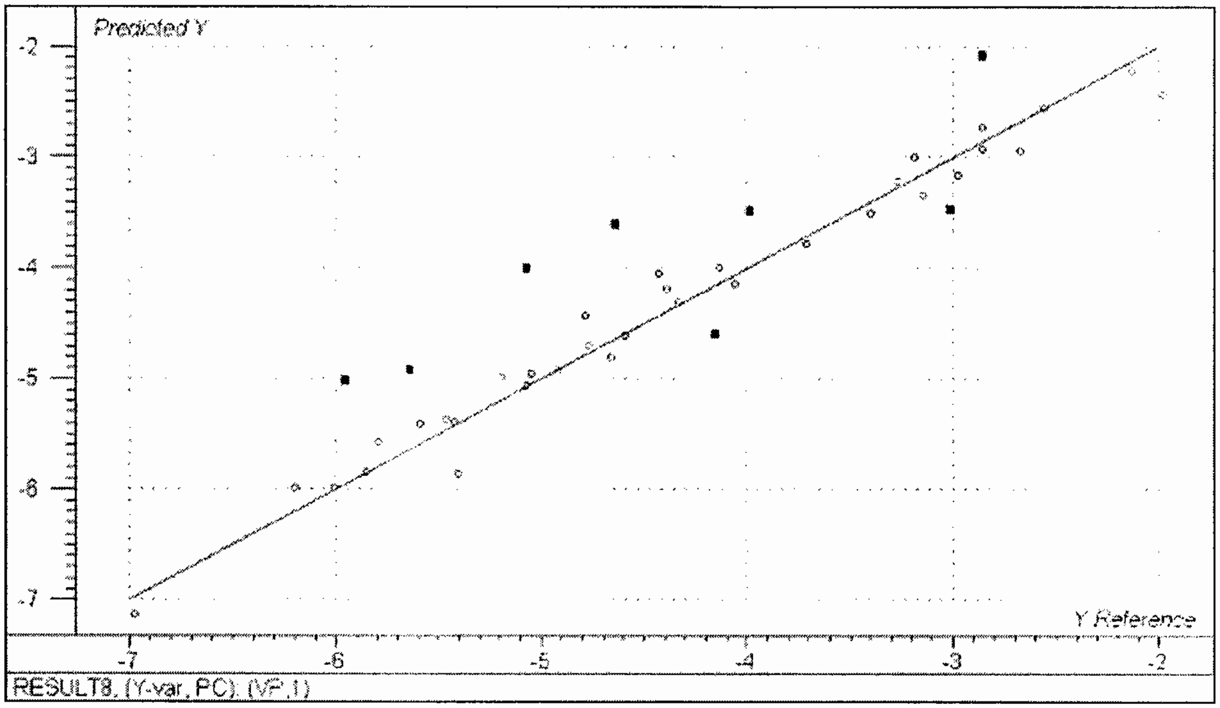

Figure 2
Predicted vs. measured vapor pressure (log mm Hg), 42 PCB congeners.

The antilogarithms of the measured and the predicted vapor pressures at 25° C (mm Hg) for all congeners, and the accompanying residuals, are listed in the enclosed tab separated text file vp.txt.

Water solubility

Experimental measurements were available for 122 congeners. Outlying objects were identified using the robust PCR procedure described above. 119 objects (objlist2.txt) and 275 descriptor variables (varlist2.txt) were assigned non-zero weight in the successive PLSR1-regression. The calibration model was validated using a test set of 47 randomly selected objects (testset2.txt). The number of latent variables to keep in the PLS-model was estimated to one, yielding a model with a coefficient of determination R^2 for the test set of 0.941. The standard error of prediction SEP, estimated from the test set, was 0.33 (log mg/l). Figure 3 show predicted versus measured results for all 122 congeners, with the three outlying objects marked as filled rectangles.

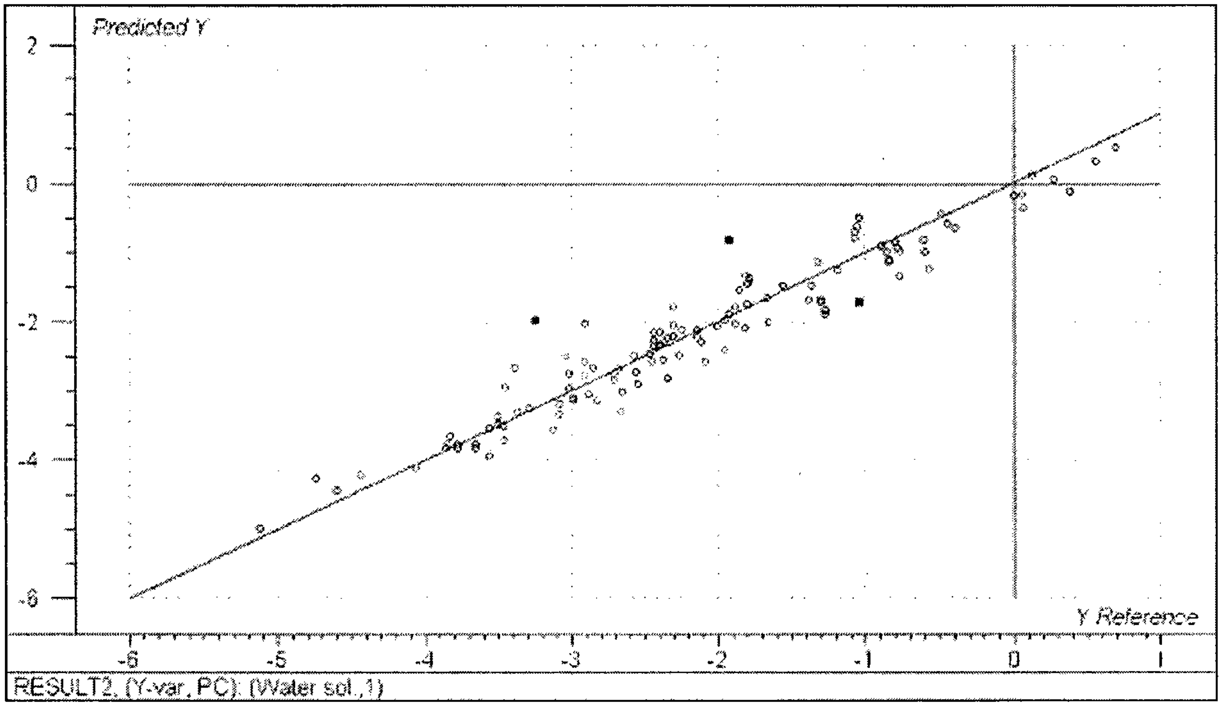

Figure 3
Predicted vs. measured water solubility (log mg/l), 122 PCB congeners.

The antilogarithms of the measured and the predicted water solubilities at 25° C (mg/l) for all congeners, and the accompanying residuals, are listed in the enclosed tab separated text file water.txt.

Partitioning coefficient octanol-water

Experimental measurements were available for 92 congeners. Outlying objects were identified using the robust PCR procedure described above. 87 objects (objlist3.txt) and 227 descriptor variables (varlist3.txt) were assigned non-zero weight in the successive PLSR1-regression. The calibration model was validated using a test set of 34 randomly selected objects (testset3.txt). The number of latent variables to keep in the PLS-model was estimated to one, yielding a model with a coefficient of determination R^2 for the test set of 0.983. The standard error of prediction SEP, estimated from the test set, was 0.15 (log P). Figure 4 show predicted versus measured results for all 92 congeners, with the five outlying objects marked as filled rectangles.

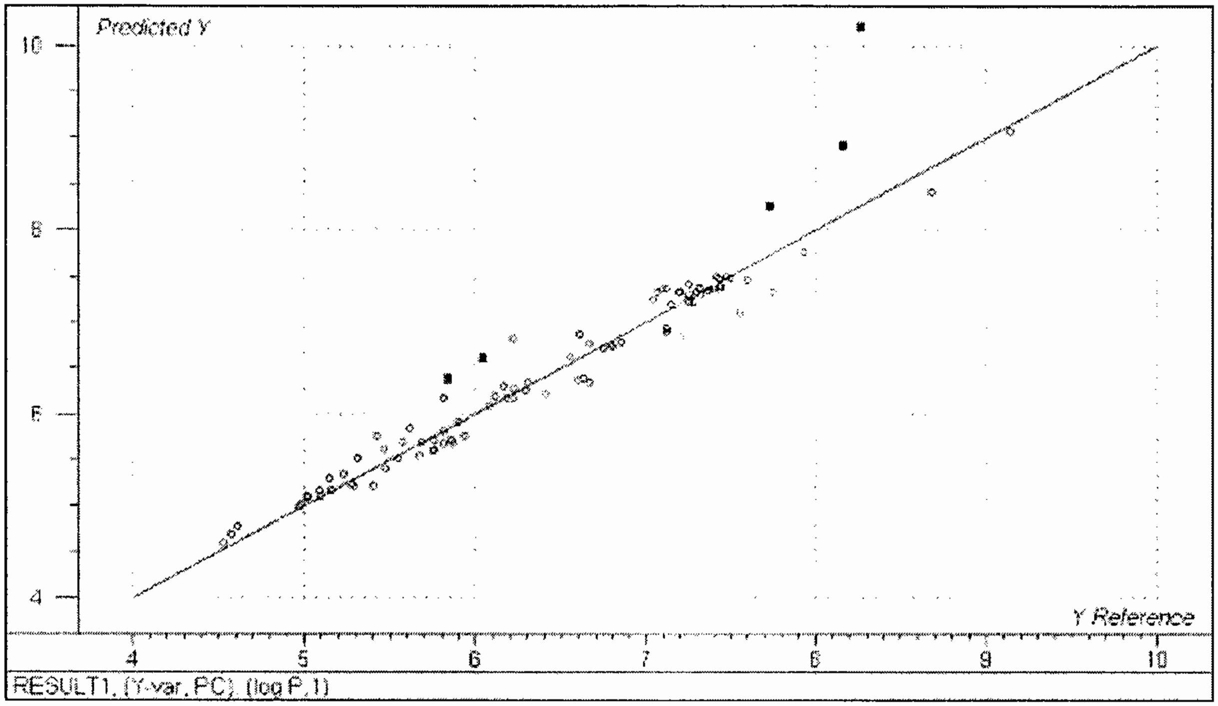

Figure 4
Predicted vs. measured partitioning coefficient octanol-water (log P), 92 PCB congeners.

The logarithms of the measured and the predicted partitioning coefficients octanol-water (log P) for all congeners, and the accompanying residuals, are listed in the enclosed tab separated text file logp.txt.

Henry's law constant

Experimental measurements were available for 91 congeners. Outlying objects were identified using the robust PCR procedure described above. 79 objects (objlist4.txt) and 145 descriptor variables (varlist4.txt) were assigned non-zero weight in the successive PLSR1-regression. The calibration model was validated using a test set of 31 randomly selected objects (testset4.txt). The number of latent variables to keep in the PLS-model was estimated to two, yielding a model with a coefficient of determination R^2 for the test set of 0.960. The standard error of prediction SEP, estimated from the test set, was 0.086 (log atm-m^3/mol). Figure 5 show predicted versus measured results for all 91 congeners, with the twelve outlying objects marked as filled rectangles.

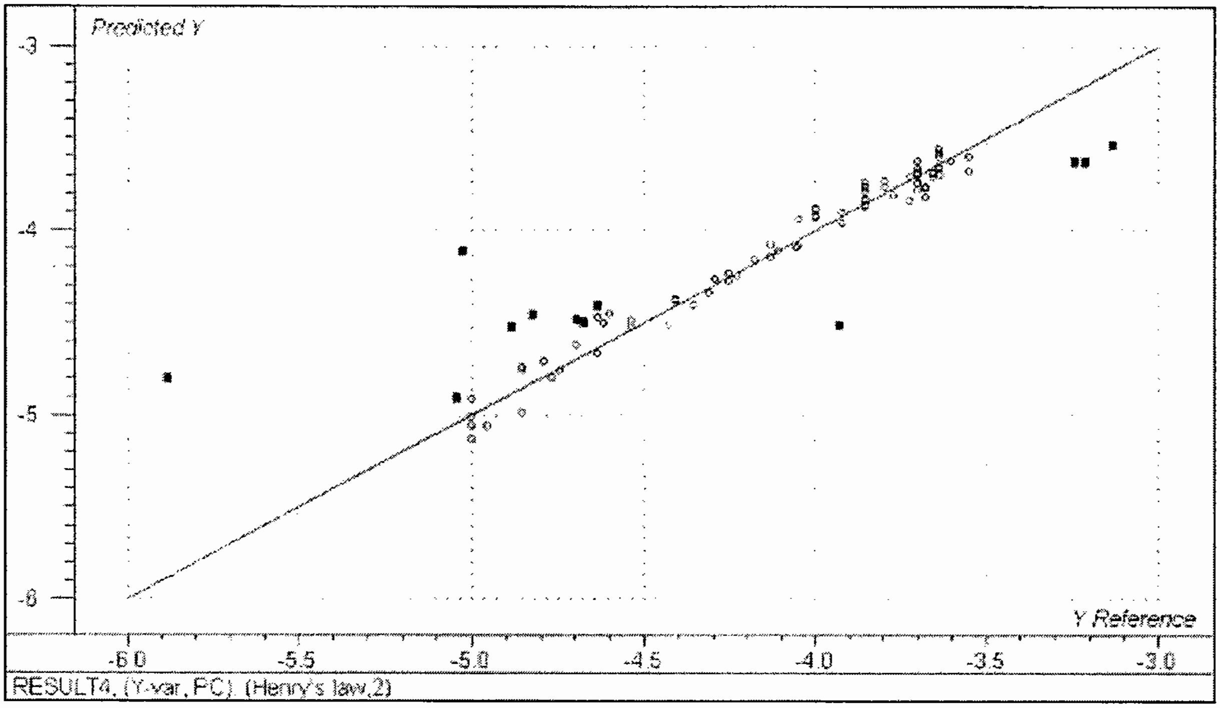

Figure 5

Predicted vs. measured Henry's law constant (log atm-m^3/mol), 91 PCB congeners.

The antilogarithms of the measured and the predicted Henry's law constants at 25° C (atm-m^3/mol) for all congeners, and the accompanying residuals, are listed in the enclosed tab separated text file henry.txt.

Retention times in gas chromatography

As an additional validation of this approach to establish quantitative structure property relationships (QSPR) for PCB congeners we have also tried to model the retention times obtained from gas chromatographic separation on three different columns: Rtx-CLP, SPB-Octyl and HT8.

Experimental measurements were available for 207-209 congeners. The retention times on all three columns showed a high correlation in between. 209 objects and 201 descriptor variables were assigned non-zero weight in PLSR2-regression. The calibration model was validated using a test set of 82 randomly selected objects. The number of latent variables to keep in the PLS-model was estimated to two, yielding a model with coefficients of determination R^2, for the test set, between 0.979 and 0.989. The standard error of prediction SEP, estimated from the test set, was 0.086-1.17 (min). Figure 6 show predicted versus measured results for 207 congeners separated on the HT8 column.

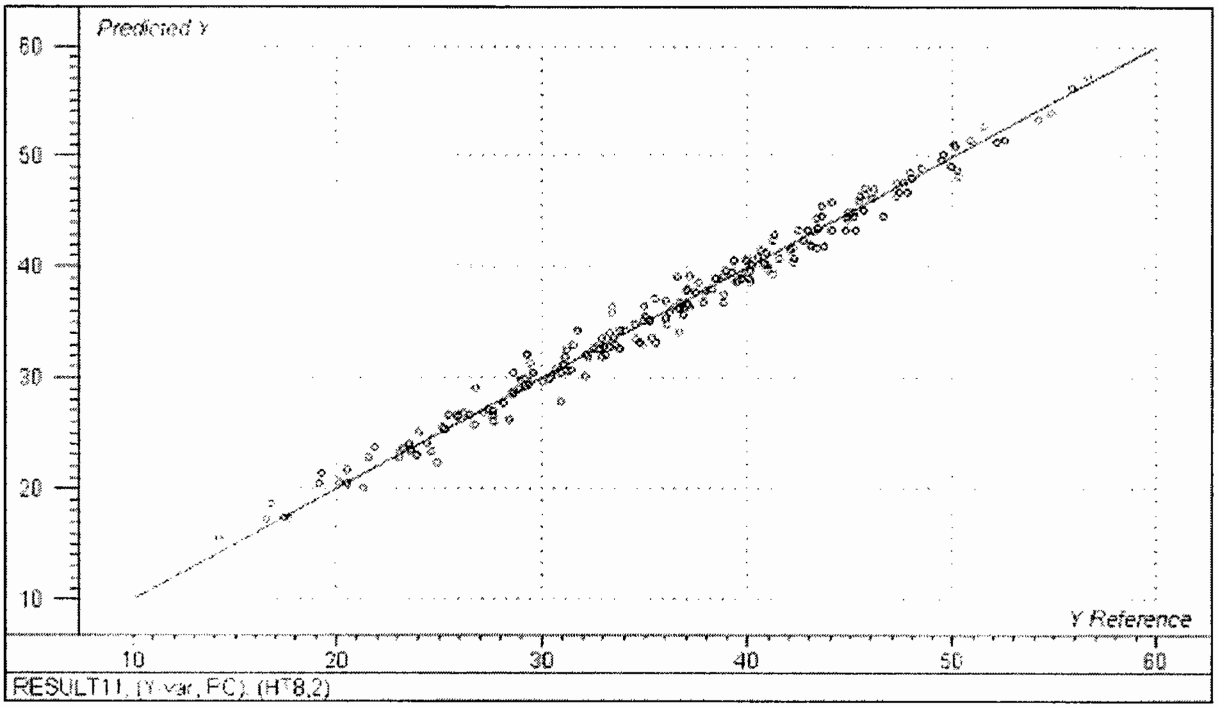

Figure 6
Predicted vs. measured retention times (min), 207 PCB congeners on a HT8 column.

The four physical properties were best described by constitutional and topological descriptors, molecular walk counts, WHIM and GETAWAY descriptors. The retention times correlated with descriptors from all groups

The results presented above shows that it is possible to obtain a good fit and low prediction errors using multivariate calibration models for physical properties, and retention times on gas chromatography columns, based solely on computationally derived descriptors. Experimental data with the smallest expected experimental errors were also the easiest to model, i.e. the retention times.

Deviation between measured values and model predictions can be due either to model error or experimental error. The "experimental error" result from both intra- and inter-laboratory variation, and especially the last factor is important since different laboratories often have used different methodology. We feel that there are rather strong indications that the experimental error is the limiting factor for these structure-property modeling efforts, since the model fit improves both with a robust approach and with more reliable data. Others have reported a similar experience with some of the group contribution methods for estimation of the partitioning coefficient octanol-water[29].

The deviation between experimental measurements and model predictions are particularly pronounced for two objects with regard to the Henry's law constant. PCB #77 and #172 have predicted values of 1.0E-4 and 1.8E-5 atm-m3/mol. The reported experimentally determined values in the PhysProp database are 9.4E-6 respectively 1.3E-6 atm-m^3/mol. We therefore made a check with the original papers, where the reported data for PCB #77 and #172 actually are a magnitude higher 9.4E-5 and 1.3E-5 atm-m^3/mol[30,31]. The large deviations are obviously due to errors in the transfer between the published data and the PhysProp database.

Validation is a general problem when using data compiled from many different sources. The usual approach to this problem is to carefully re-evaluate all original data and investigations. However, in many cases this can prove to be difficult and at least very time consuming. Furthermore, experimental errors will often remain after this process. Another way of dealing with the problem is to use high-breakdown methods for data evaluation, i.e. robust methods for model building that can accept significant contamination with bad data. Least median of squares regression is an example of such a robust method, with a breakdown point of 50%. This method will work if we can expect at least 50% "good data", and this does seem as a conservative assumption in many practical situations.

How reliable are then the model predictions compared to the individual experimentally determined results? Each model interpolation is actually based on a substantial number of experiments performed in various laboratories. We are therefore inclined to put more faith in the model interpolations if a reported experimental value show up as an outlier with a high residual. It will be very interesting to see if repeated measurements on some of the congeners with the largest reported deviations will provide a more definitive answer to this.

Conclusions

We have in this investigation reported estimations of some important basic physical parameters for all 209 congeners of polychlorinated biphenyls. These estimations were made from computationally derived descriptors using a robust approach to multivariate calibration. In a number of cases large deviations were detected from the reported experimentally determined values. Some of these could directly be assigned to typing errors. The most reliable measurements available, retention times from gas chromatography, were also the easiest to predict with accuracy and precision. The model predictions therefore seem to provide a reliable summary and extension of the currently available database on these compounds.

Supplementary materials

- List of descriptor variables generated by the software Dragon as a text file.
- List of descriptor variables used in this study as a text file.
- Raw data file with descriptor and response variables as a tab separated text file.
- Score vectors from PCA as a tab separated text file.
- Text files with lists of objects (congeners), descriptor variables and test set for the vapor pressure PLS regression model.
- Measurements, predictions and residuals for vapor pressure (mm Hg) as a tab separated text file.
- Text files with lists of objects (congeners), descriptor variables and test set for the water solubility PLS regression model.
- Measurements, predictions and residuals for water solubility (mg/l) as a tab separated text file.

- Text files with lists of objects (congeners), descriptor variables and test set for the partitioning coefficient PLS regression model.
- Measurements, predictions and residuals for partitioning coefficient octanol-water (log P) as a tab separated text file.
- Text files with lists of objects (congeners), descriptor variables and test set for the Henry's law constant PLS regression model.
- Measurements, predictions and residuals for Henry's law constant (atm-m^3/mol) as a tab separated text file.

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SWEDISH EnviroNet

APPENDIX D

FUGACITY EQUATION SUBSTITUTIONS

Individual fugacities for each compartment (as a bulk media) are described by the following equations:

(Air)

$$f_1 = \frac{D_{21} f_2}{D_{12} + DA_1} = \frac{D_{21} f_2}{DT_1} \text{ (no reaction in air)}$$

(Upper water column)

$$f_2 = \frac{D_{32} f_3 + D_{12} f_1}{D_{21} + D_{23} + D_{A2} + D_{R2}} = \frac{D_{32} f_3 + D_{12} f_1}{DT_2}$$

(Lower water column)

$$f_3 = \frac{D_{53} f_5 + D_{23} f_2 + D_{43} f_4}{D_{32} + D_{34} + D_{A3} + D_{R3}} = \frac{D_{53} f_5 + D_{23} f_2 + D_{43} f_4}{DT_3}$$

(Sediment Bed)

$$f_4 = \frac{D_{34} f_3}{D_{43} + D_{R4} + D_B} = \frac{D_{34} f_3}{DT_4}$$

(Vessel Interior)

$$f_5 = \frac{N_5}{D_{A5}}$$

Direct substitution to solve for f_2 as a function of f_3:

$$f_1 = \frac{D_{21} f_2}{DT_1}$$

$$DT_2 f_2 = D_{32} f_3 + D_{12} \times \frac{D_{21} f_2}{DT_1}$$

$$DT_2 f_2 - \frac{D_{12} D_{21} f_2}{DT_1} = D_{32} f_3$$

$$f_2 \left(DT_2 - \frac{D_{12} D_{21}}{DT_1} \right) = D_{32} f_3$$

$$f_2 = \frac{D_{32} f_3}{DT_2 - \frac{D_{12} D_{21}}{DT_1}}$$

Direct substitution to solve for f_3:

$$f_4 = \frac{D_{34} f_3}{DT_4}$$

$$DT_3 f_3 = D_{53} f_5 + \frac{D_{23} D_{32} f_3}{DT_2 - \frac{D_{12} D_{21}}{DT_1}} + \frac{D_{43} D_{34} f_3}{DT_4}$$

$$DT_3 f_3 = D_{53} f_5 + f_3 \left(\frac{D_{23} D_{32}}{DT_2 - \frac{D_{12} D_{21}}{DT_1}} + \frac{D_{43} D_{34}}{DT_4} \right)$$

$$DT_3 f_3 - D_{53} f_5 = f_3 \left(\frac{D_{23} D_{32}}{DT_2 - \frac{D_{12} D_{21}}{DT_1}} + \frac{D_{43} D_{34}}{DT_4} \right)$$

$$\frac{DT_3 f_3}{f_3} - \frac{D_{53} f_5}{f_3} = \frac{f_3}{f_3} \left(\frac{D_{23} D_{32}}{DT_2 - \frac{D_{12} D_{21}}{DT_1}} + \frac{D_{43} D_{34}}{DT_4} \right)$$

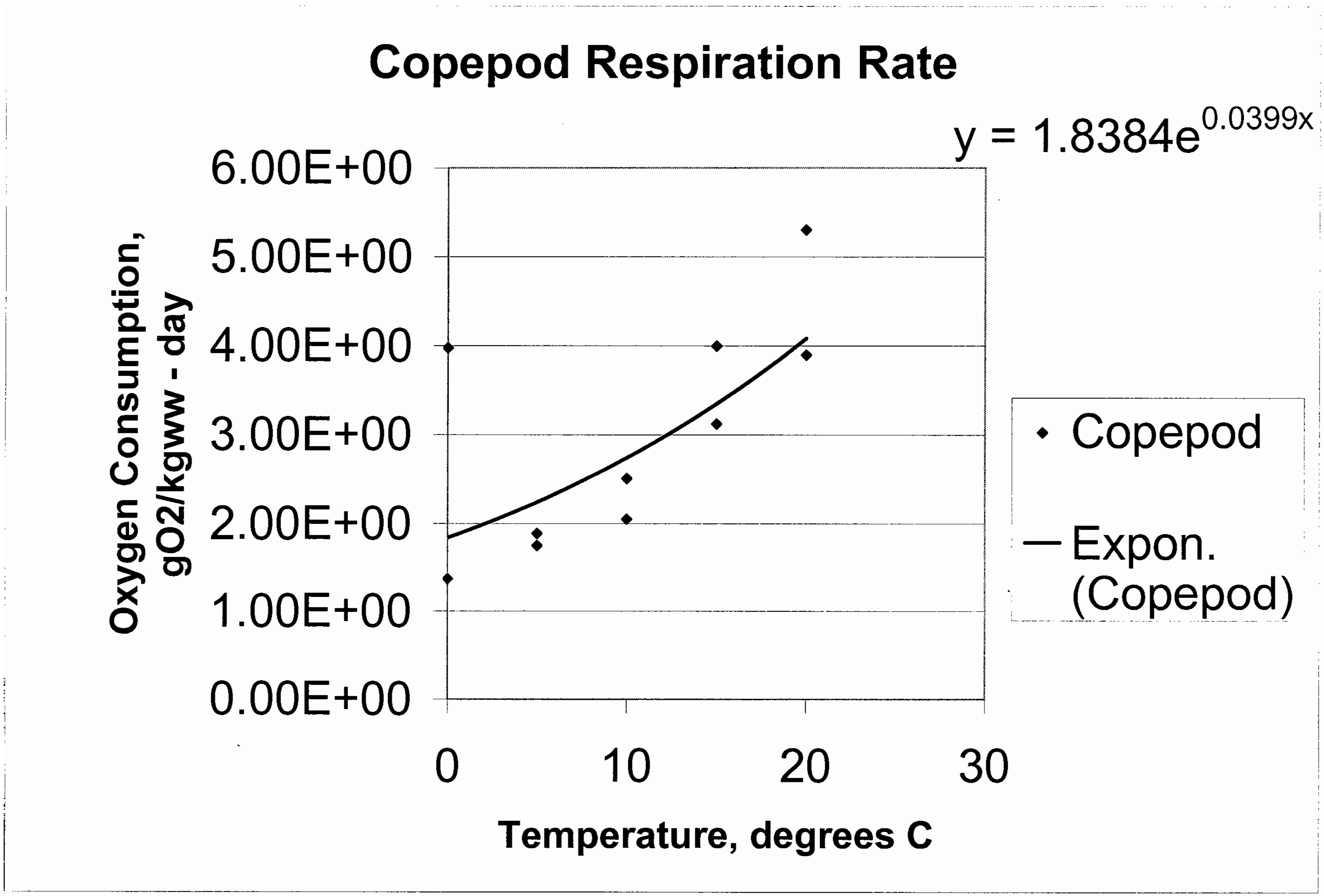
$$DT_3 - \frac{D_{23} D_{32}}{DT_2 - \frac{D_{12} D_{21}}{DT_1}} - \frac{D_{43} D_{34}}{DT_4} = \frac{D_{53} f_5}{f_3}$$

$$f_3 = \frac{D_{53} f_5}{DT_3 - \frac{D_{23} D_{32}}{DT_2 - \frac{D_{12} D_{21}}{DT_1}} - \frac{D_{43} D_{34}}{DT_4}}$$

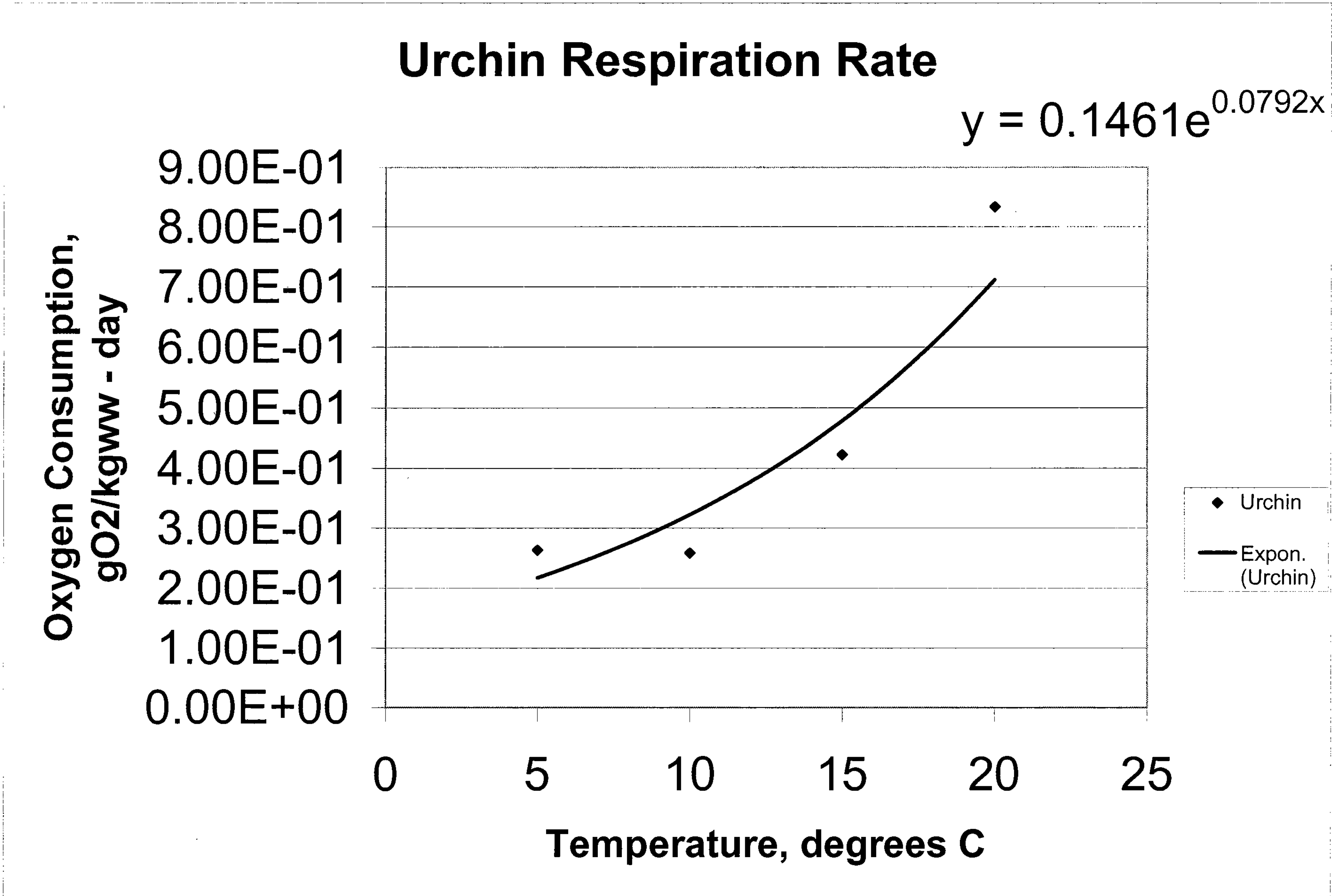
$$f_3 = \frac{D_{53} f_5}{DT_3 - \frac{D_{23} D_{32} DT_1}{DT_1 DT_2 - D_{12} D_{21}} - \frac{D_{34} D_{43}}{DT_4}}$$

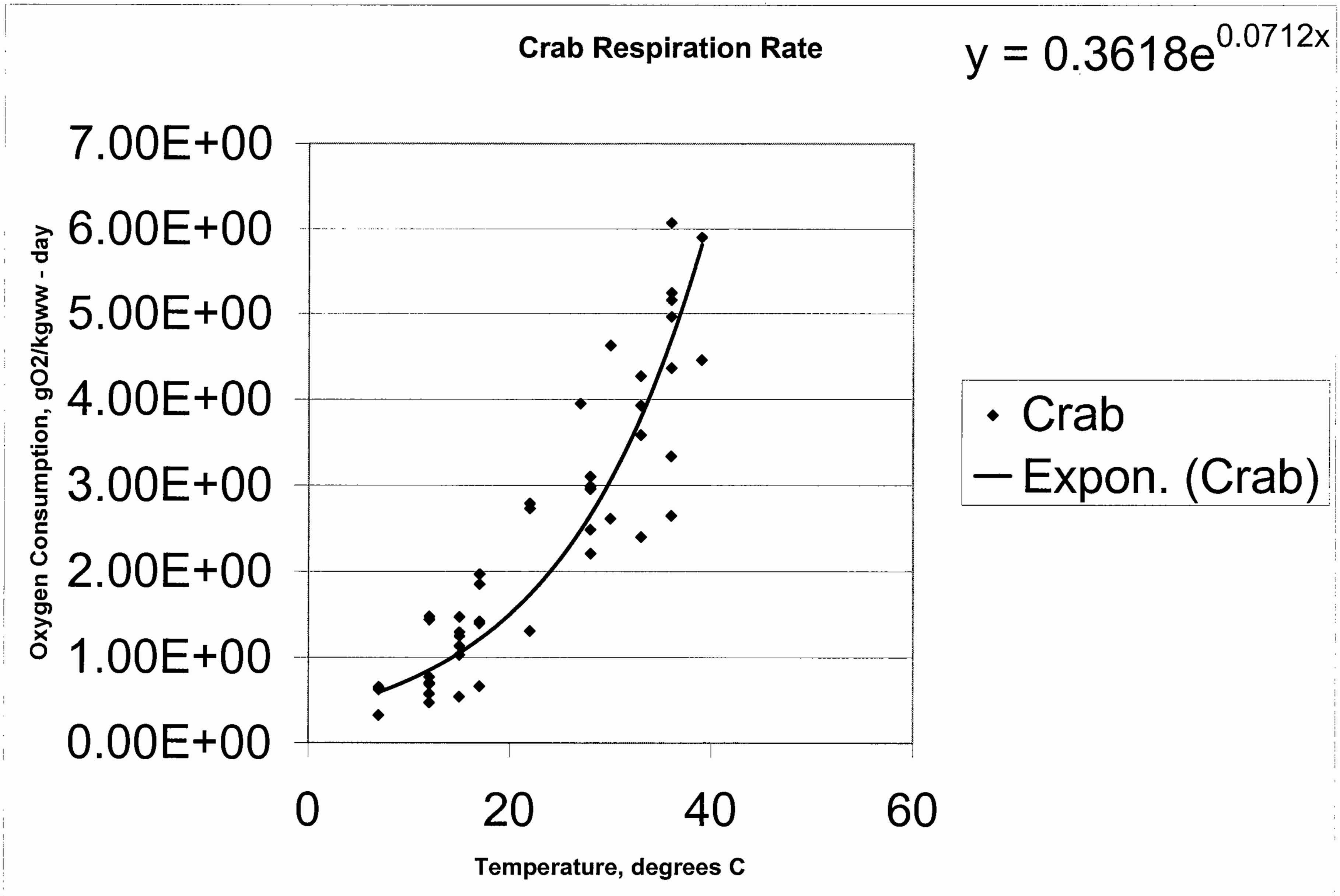
APPENDIX E

ORGANISM RESPIRATION REGRESSIONS

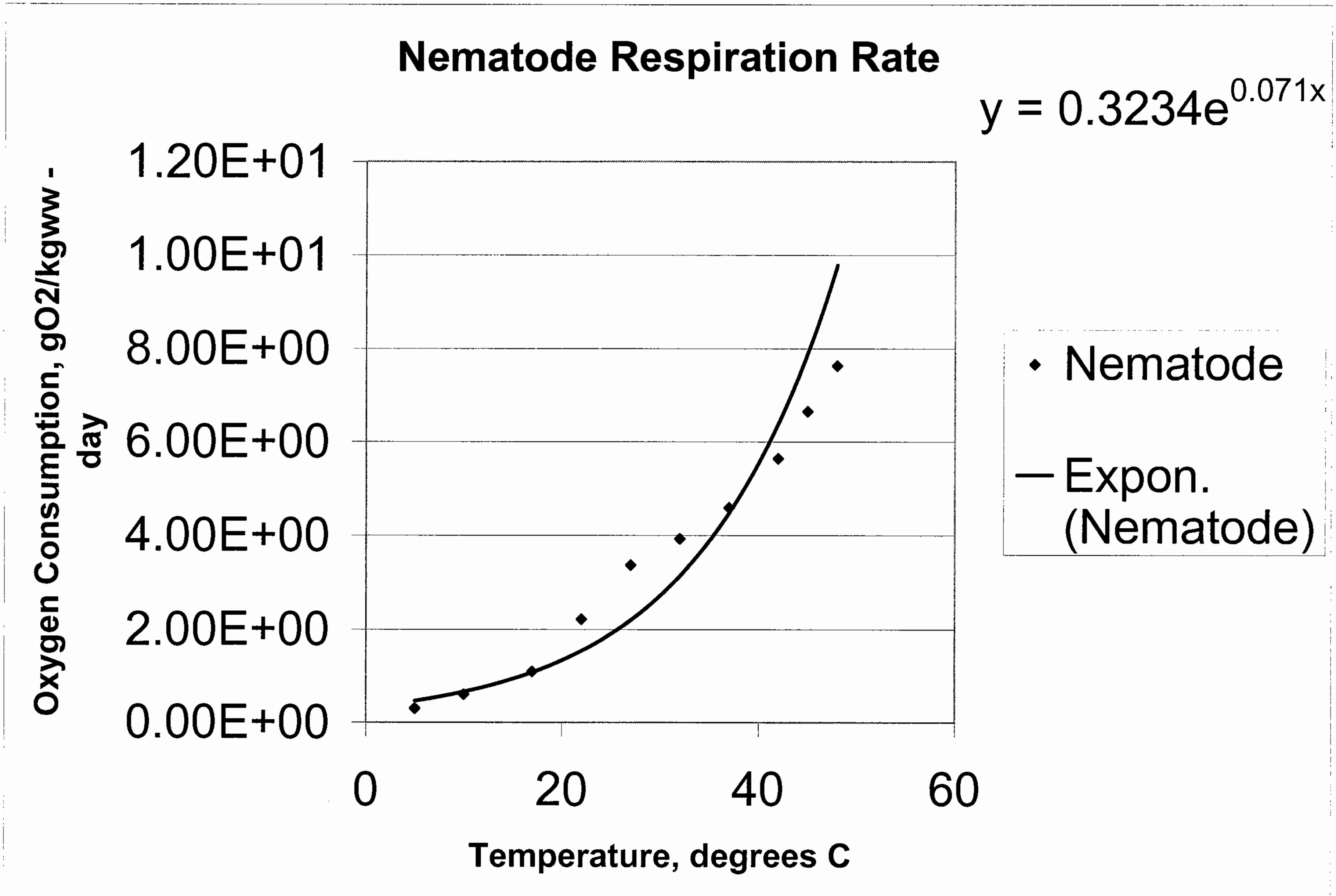


I:\Projects\PRAM\33756123 Navy PCB HHRA_WP\03000\REPORT\PRAM_ORISKANY-APP J.xls\Copepod Chart 1


Urchin Respiration Rate
y = 0.1461e^0.0792x
Oxygen Consumption, gO2/kgww - day
9.00E-01
8.00E-01
7.00E-01
6.00E-01
5.00E-01
4.00E-01
3.00E-01
2.00E-01
1.00E-01
0.00E+00
0
5
10
15
20
25
Temperature, degrees C
Urchin
Expon. (Urchin)



Crab Respiration Rate
$y = 0.3618e^{0.0712x}$
7.00E+00
6.00E+00
5.00E+00
4.00E+00
3.00E+00
2.00E+00
1.00E+00
0.00E+00
Oxygen Consumption, gO2/kgww - day
0
20
40
60
Temperature, degrees C
Crab
Expon. (Crab)



I:\Projects\PRAM\33756123 Navy PCB HHRA_WP\03000\REPORT\PRAM_ORISKANY-APP J.xls\Nematode Chart 1

APPENDIX F

ZONE OF INFLUENCE

This appendix is intended to provide additional details about the potential composition of a fish assembly that might be associated with the artificial reef ex-ORISKANY, and information of relevance to establishing spatial boundaries of that assemblage.

In plan view, the "footprint" of the ex-ORISKANY vessel is about 10,000 square meters (m^2), or a hectare (2.5 acres). Assuming that the vessel comes to rest in an upright attitude and minimally penetrates the substrate, most of the structure will extend about 30 meters (m) upward through the water column, with a portion (the "island") extending another 15 m (to within about 15 m of the sea surface). The vessel will provide about 27,800 m^2 (nearly 7 acres) of surface, which is likely to be perceived by marine organisms as the structural equivalent of "hard bottom" (Department of the Navy, 2004). There are scattered natural hard-bottom habitats in the general vicinity of the proposed site (i.e., within a few tens of kilometers [km]), but the main concentrations of such structures are at least 80 km to the southwest, and predominantly in deeper water (Thompson et al., 1999; Weaver et al., 2002). Thus the ex-ORISKANY will present an ecological novelty.

Inasmuch as fishers and aquatic ecologists have known for centuries that many fishes and other nektonic animals tend to congregate near submerged structures, both natural and artificial, (e.g., Walton, 1976; Moyle and Cech, 1982), it is reasonable to assume that from the potential "pool" of nektonic animals in the northeastern Gulf of Mexico there will be a subset that associates with the ex-ORISKANY. The issue becomes which kinds ("species"), to what degree (spatially and temporally), and in what densities nektonic assemblages will occur at the artificial reef. There are at least 300 kinds of fish, known or presumed to represent formally described (named) species, which have been recorded in waters overlying the northeastern Gulf of Mexico continental shelf between Longitudes 85° and 88° at depths from 15 to 70 m (~49 to ~230 feet). The foregoing statement is based on review of lists compiled from various sources, including Hoese and Moore (1998), Thompson et al. (1999), Weaver et al. (2002), Carpenter (2002), and others. At least some individual representatives of many of the aforementioned 300-plus fish species may spend various increments of time in a particular location such as that of the proposed site of the ex-ORISKANY.

The Gulf of Mexico Fishery Management Council (GMFMC, 2003) recognizes the following species as reef fish for purposes of its management planning:

Common Name	Species
Gray triggerfish	*Balistes capriscus*
Greater amberjack	*Seriola dumerili*
Lesser amberjack	*Seriola fasciata*
Almaco jack	*Seriola rivoliana*
Banded rudderfish	*Seriola zonata*
Hogfish	*Lachnolaimus maximus*
Queen snapper*	*Etelis oculatus*
Mutton snapper**	*Lutjanus analis*
Schoolmaster snapper**	*Lutjanus apodus*
Blackfin snapper	*Lutjanus bucanella*
Red snapper	*Lutjanus campechanus*
Cubera snapper**	*Lutjanus cyanopterus*
Gray snapper	*Lutjanus griseus*
Dog snapper	*Lutjanus jocu*
Mahogany snapper**	*Lutjanus mahogoni*
Lane snapper	*Lutjanus synagris*
Silk snapper*	*Lutjanus vivanus*
Yellowtail snapper+	*Ocyurus chrysurus*
Wenchman	*Pristipimoides aquilonaris*
Vermilion snapper++	*Rhomboplites aurorubens*
Blueline tilefish	*Caulolatilis microps*
Tilefish*	*Lopholatilis chamaeleonticeps*
Rock hind	*Epinephelus adscensionis*
Speckled hind	*Epinephelus drummondhayi*
Yellowedge grouper*	*Epinephelus flavolimbatus*
Red hind	*Epinephelus guttatus*
Goliath grouper (formerly jewfish)	*Epinephelus itajara*
Red grouper	*Epinephelus morio*
Warsaw grouper	*Epinephelus nigritus*
Snowy grouper*	*Epinephelus niveatus*
Nassau grouper+	*Epinephelus striatus*
Black grouper	*Mycteroperca bonaci*
Yellowmouth grouper	*Mycteroperca interstitialis*
Gag (or gag grouper)	*Mycteroperca microlepis*
Scamp	*Mycteroperca phenax*
Yellowfin grouper**	*Mycteroperca venenosa*

* Adults may tend to avoid ex-ORISKANY because site is too shallow (GMFMC, 2003); Yellowedge grouper (*Epinephelus flavolimbatus*) and Snowy grouper (*Epinephelus niveatus*) were added to this group of fish per personal communication with Jon Dodrill, Florida FWCC, 01/05/05).

** Adults may tend to avoid ex-ORISKANY because site is too deep (GMFMC, 2003).

\+ Proposed site is outside normal geographic range (Carpenter, 2002).

++ Addition to the above GMFMC table per personal communication with J Dodrill, Florida FWCC, 01/05/05).

There is a good chance that adult individuals of species not footnoted (as "*" or "**") in the above list will eventually be recorded at the ex-ORISKANY site, and a few (e.g., gray triggerfish, red snapper, gag) are likely to become effectively "resident" and contribute significantly to local fishery landings. Many additional species will probably establish effective residence (as juveniles and adults), a few of which are not formally managed by the GMFMC as 'reef fish' (e.g., tomtate [*Haemulon aurolineatum*]) but are nevertheless exploited by fishers. Even so, the vast majority of the fishes that will spend most of their lives at the vessel are relatively small and/or of little or no interest to anglers. Examples of such "non-fishery" obligate reef fishes are wrasses, grunts, blennies, sandbasses, and gobies; these fish will be relevant to the ecological risk assessment (and as prey for some of the fishery species).

For purposes of the Prospective Risk Assessment Model (PRAM), only a few representatives of the 30 or so species likely to be associated with the vessel, and likely to be eaten by humans, are of special interest. That is, which among the fishery species are likely to have representatives that spend a substantial fraction of their lives (multiple years, in aggregate) in close proximity to the ex-ORISKANY?[1] Based on anticipated behavior, how many different types of fish are expected to have substantial affinity to the vessel?

[1] None of the fishery species likely to occur at the ex-ORISKANY spends its entire life in one location. These fishes often spawn in areas other than where they forage; and they all have planktonic larvae which in most cases "settle" in inshore areas where they spend a few to many months before moving offshore (Carpenter, 2002; GMFMC, 2003). Some of the larger fishes (e.g., most groupers) tend to migrate to progressively deeper water in the later years of their lives (Carpenter, 2002; GMFMC, 2003). Also, many of the larger predatory fishes may be removed by anglers within the first year or so after they first arrive at ex-ORISKANY (J. Dodrill, Florida FWCC, personal communication, 1/5/05). All of these realities are ignored by the PRAM (i.e., the model conservatively assumes that the fish remain consistently within the Zone of Influence [ZOI] throughout their lives).

There are two basic behavioral scenarios in the context of the PRAM. There are fishes that focus their foraging on vertical (or "suspended" horizontal) substrates, and thus would move up and down along the sides of ex-ORISKANY (e.g., gray triggerfish). This behavior entails gleaning or grazing on encrusting organisms and small animals living in or on the encrusted colonies (Beaver, 2004). The other basic behavior involves preying on plankton, smaller nekton (than the predator), and or benthic invertebrates associated with the sea bottom lateral to the vessel (e.g., red snapper). The second behavior involves substantial movement within the water column, at least while feeding (which is what most fish do when not resting or spawning [Moyle and Cech, 1982; Gerking, 1994). Practitioners of the second behavior may spend most of their time at various levels within the water column above the seafloor, and are traditionally referred to as *pelagic* (e.g., amberjacks), and some may spend most of their time very near or in contact with the natural bottom (called *demersal*; e.g., tilefish, some snappers and groupers). Still others may forage more or less equally in the water column and along the seafloor (e.g., some snappers and grunts).

To satisfy the requirements of PRAM to model PCB fate and transport in the abiotic media and to model trophic transfer of PCBs, it is necessary to identify the external boundary of at least one Zone of Influence (ZOI). However, in the context of evaluating human health risk associated with consumption of fish, it may be advantageous to consider using at least two different ZOIs to account for the above behavioral scenarios of fish. From the perspective of an aquatic ecologist this simply equates to identifying a realistic, albeit conservative, increment of space (distance) from the external surface of the ex-ORISKANY that would allow a fish to perform its behavior.

In the case of the gray triggerfish (*B. capriscus*) the estimate is relatively straight-forward. Because of its unusual mouth structure, a triggerfish is constrained to feed at a roughly perpendicular orientation relative to the surface on which it is grazing (Gerking, 1996). Since the typical adult *B. capriscus* is roughly 20 centimeters (cm) in total length (Hoese and Moore, 1998), one might suggest that the minimal, (most conservative) space, to allow at least some maneuverability is 0.5 m. However, a space as small as a fraction of a meter is unrealistic for use as a ZOI. This distance is only related to maneuverability for feeding, and does not account for other factors, such as opportunistic feeding behavior (Harper and McClellan, 1997). Triggerfish commonly feed on benthic invertebrates in the sediment bed adjacent to the reef, as well as encrusting organisms on the reef surface. Turpin (personal communication, 2005)[2] notes that reef-associated triggerfish commonly range more than10 m from the reef as part of their foraging behavior. This observation is consistent with information provided in Bortone et al. (1998) demonstrating a high level of predation of benthic organisms in the vicinity of artificial reefs, with maximum impacts on benthic biomass occurring between10 and 20 meters from the reef, as well as the observation that anglers regularly catch triggerfish several meters away from structures (personal experience and testimony of others). In addition to the above considerations, when determining which ZOI boundaries may be appropriate, one must also consider that within the PRAM, the ZOI also defines the volume into which PCBs released from the sunken vessel are received. PRAM uses an artificial construct of the sunken vessel, which assumes that all of the bulkheads of the vessel are porous, and do not retard the release of PCBs into the ZOI. To the extent that this does not accurately characterize the manner in which PCBs will be released from the vessel (i.e., PCBs may actually emanate from discrete apertures or "leakage" areas), an adequate distance around the sunken vessel should be assumed such that PCB release and distribution can occur. Therefore, a minimal distance of 15 meters is recommended to evaluate exposure to near-field foraging fishes such as triggerfish.

For the pelagic and demersal behavior scenarios the estimate is more complex. Ideally, one would have copious detailed observations of individually recognizable (or tagged) individuals representing at least a few anticipated fishery species. For the probable ex-ORISKANY examples mentioned above, there do not appear to be any such studies over short time periods at a local scale. There are some local-scale studies for fishes associated with natural reefs. In one example using acoustic telemetry, the Bermuda chub (*Kyphosus sectatrix*) was found to have elongate home ranges with lengths of 157-1259 meters and widths of 54-234 meters (Eristhee and Oxenford, 2001). That is, of the 11 tagged individuals tracked over a two-month period, there was one fish that limited its movement in one dimension to 54 meters. Regional-scale tagging studies are of little relevance to the immediate issue, because they generally tend to focus on questions about how far fish travel in the context of migration over extended periods. In such studies, many re-captures are recorded as occurring literally at the point of release (mainly early in the overall study) and the less frequent re-captures at remote locations are on the scale of tens or even hundreds of kilometers. Several such studies have been performed on red snappers in various parts of the

[2] Personal communication from Robert Turpin, Escambia County, Florida Marine Resources Division (01/05/05). Gray triggerfish associated with artificial reefs are opportunistic feeders that commonly feed on encrusting organisms on reefs and on benthic organisms in the vicinity of reefs. Based on personal observations on numerous artificial reef sites, gray triggerfish are commonly seen foraging on benthic organisms more than 10 meters from reef structures (often 40 meters or more).

Gulf of Mexico, some of which indicated a high rate of "fidelity" to the location of release, but virtually all of the cases had some records indicating movements on the scale of tens of (or more) kilometers (Fable, 1980; Szedlmayr and Shipp, 1994; Patterson et al., 2003; and others).

Recent development of multi-beam hydroacoustic technology has provided some valuable insights into the probable magnitude of local movements of pelagic and demersal artificial-reef associated fishes (Stanley, 1994; Stanley and Wilson, 1996, 1997, 1998, 2000a, b, 2003; Wilson et al., 2003). Some of the earlier of these studies merely indicated fish assemblage density discontinuities, thereby defining the boundaries of aggregations at the times of observations. More recently, the work has become much more sophisticated by deployments of stationary equipment that is capable of distinguishing the specific types of fish comprising a given aggregation. Studies have also captured data among a variety of submerged structure types (including petroleum platforms, artificial reefs, and natural hard-bottom habitats) and from different seasons.

The hydroacoustic studies have revealed two basic types of information of relevance to the ex-ORISKANY ZOI dimensions:

- Patterns of density magnitude vary substantially among seasons, indicating that at a fixed location at least some individuals are not always present.
- Spatial boundaries of aggregations (density discontinuities) are relatively similar at a given submerged structure, and they suggest localized short-term (on the scale of hours or less) movements within a range of tens of meters. Over a range of different structures, the span of distances to apparent aggregation 'boundaries' (relative to the structures) was about 12 to 50 m.

Using the results of one of the later studies at a petroleum platform in a bathymetric setting similar to that of the proposed ex-ORISKANY site, Stanley and Wilson (2003) estimated a 'near-field' area of influence of 18 meters. This distance was consistent with standard estimates derived from videographic surveys performed via remotely operated underwater vehicles (ROVs). It is also of interest to note that Bortone et al. (1998) found that demersal reef fish tended to measurably affect the composition and abundance of infaunal benthic communities out to distances as great as 80 m (see also Lindquist et al., 1994). However, in the Bortone et al. (1998) study the typical distance at which several benthic community metrics seemed to reflect a reversal in the pattern of disturbance was in the range of 10 to 20 m.

Based on the foregoing, it seems reasonable to suggest that the 'near-field' area of influence observed by Stanley and Wilson (2003) should provide a basis for a conservative estimate of the magnitude of the ZOI for the PRAM as applied to the ex-ORISKANY, whereas a distance of 50 to 80 meters, consistent with the disturbance patterns noted by Bortone et al. (1998) and Lindquist et al. (1994) should provide an upperbound estimate of the ZOI boundaries. This would apply particularly for the pelagic and demersal fishes that clearly would not obtain the bulk of their diets from the surface of the vessel itself.

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APPENDIX G

CLARIFICATIONS/ADDITIONS AND RESPONSES TO BIOLOGY TWG COMMENTS ON NAVY ENVIRONMENTAL HEALTH CENTER (NEHC) PROPOSED FOOD WEB DIET – WATER EXPOSURE MATRIX

Clarifications/Additions and Responses to Biology TWG Comments on Navy Environmental Health Center (NEHC) Proposed Food Web Diet –Water Exposure Matrix

January 9, 2005

All clarifications/additions, revisions, and responses are provided below the commenter's statements.

Dr. Wayne Munns Comments:

As a result of today's [12-15-04] discussion, I am in basic agreement with the approach being taken to evaluate the progression of exposures to components of a reefed vessel food web. My sense is that it will address several of the issues raised during previous reviews of PRAM and the risk assessments. I appreciate the significant effort undertaken by the Navy to address these issues, and assuming that the response to the other review comments regarding PRAM is as aggressive, I believe that this next version of PRAM will be a highly credible and flexible tool to support decisions about the Oriskany and future vessels.

Response: Thank you – comment noted.

In addition to supporting the specific modifications to values suggested by Roland, Robert T. and Bob J., I'd like to emphasize what I believe to be some key considerations as we proceed with model documentation and analyses (with apologies in advance if these are obvious):

1) The reasoning behind the choices of analysis structure and specific values should be documented. To reiterate, I don't think this means an exhaustive review of existing literature and data. Rather, sufficient rationale should be provided to facilitate understanding of those choices. If a choice was based on intuitive logic (e.g., piscivores primarily eat fish), it's likely sufficient to state that. If based on precedent (e.g., the approaches mirrors that taken by other accepted models), say so and cite the relevant precedent(s). If based on existing information and data, simply cite the sources. If due to fundamental modeling constraints (zooplankton feeding on zooplankton would lead to infinite exposure), describe the limitation. Choices based on best professional judgment are a bit more problematic, in that the underlying considerations need some description and explanation, The important thing here is to explain the reasoning used to a level at which a reasonable person can understand that reasoning. I sensed that Mark and others understood this.

Response: Comment noted. We have been working to address this in the documentation of the PRAM food web model construct. The matrix tables present findings from our review of literature, comments offered by the biology TWG members, and professional judgment.

2) Within reason, the ramifications of those choices with respect to model output should be described. This consideration was behind my question to Mark about the sensitivities of model output to parameter choices. Obviously, exhaustive formal sensitivity analyses are the gold standard here, but such are not necessary (nor does time permit).

Response: A sensitivity analysis was performed on an earlier version of the PRAM that revealed that biogenetic inputs and certain chemical inputs (e.g., Kow, Koc) were far more sensitive than dietary preferences. That analysis, however, was performed on a much simpler food chain than is currently incorporated into PRAM. With the revised foodweb in PRAM, we do agree that additional sensitivity analyses would be helpful to evaluate the potential significance of varying parameters. Given the time constraints, this effort could be considered, if so requested by the TWG, after the submission of our PRAM documentation deliverables.

The answer Mark had provided to my question is a good start, but stopping there may risk questions about the appropriateness of parameter values chosen. Somewhere in between would be multiple (i.e., more than one) model (or sub-model) runs that can serve to bound model outputs. I suspect we might want to give this issue some additional thought.

Response: We have discussed "bounding" results that may address this, using upper and lower limits of assumed values. Given the large number of variables (parameter values) required to model PCB release from the vessel, and subsequent transfer through the food web, it is unlikely that any meaningful bounding estimate could be provided. As such, we do not propose to provide bounding estimates. It is important to note that the parameter values chosen for inclusion in PRAM were based on the best available information, and have undergone review by the members of the biology Technical Working Group (TWG) in order to arrive at representative and defensible consensus values.

3) As discussed by Bill and others, the documentation should be very clear about the degree of conservatism embodied within the choices. Although I might argue that assumptions and approaches in risk assessments, even screening-level RAs, should not be conservative, others hold a different perspective (usually for good reason). The decision-makers and stakeholders will want to understand the degree of conservatism assumed as it influences their confidence that they're not making a wrong decision.

Response: Comment noted.

I think we want all parties to the decision about the ex-ORISKANY to be able to stand behind the science supporting that decision. It's to everyone's advantage to have the communication of that science be transparent.

We did not reach consensus on whether or how to address the issue of risks to organisms with exposure pathways involving the interior of the ship. As some of us had suggested, both risk assessments [Human Health and Ecological] likely will need to address this issue in some fashion.

We had discussed (at least) three options for doing this: 1) incorporating additional reef components explicitly as environmental compartments (Bob J.'s "interior reef community"), 2) modifying PRAM to allow exposure of sessile filter feeders to vessel interior waters (as represented by unshading cell D10 in the water exposures matrix), or 3) acknowledging the lack of explicit analysis in a discussion of uncertainties. Absent hard information about utilization of the ship's interior by members of the reef community, which of these options is "best" is not apparent to me. However, an approach that combines options 2 and 3 seems reasonable and defendable. Allowing the potential for exposure to be non-negative brings its consideration into the analyses explicitly, and increases the flexibility of PRAM to accommodate various assumptions about the contribution of this exposure route if need arises. When associated with a discussion of the assumed value (zero or some low percentage) and attendant uncertainties in this value and its effects on model output, people may quibble about that value, but they can't charge that the pathway was ignored. To address one of Andrea's concerns, allowing some non-negative percentage of exposure to interior waters seems to be no different than assuming various percentages of exposure to other waters (or prey) to other receptors -- these percentages are intended to represent reasonable guesstimates of exposures averaged across individuals of each of the receptor populations. Thus, this approach is consistent with that taken throughout.

Response: In order to make PRAM more flexible, we have unblocked cell D10 and have recommended a value of 0 percent, which reflects our position that a vessel interior community is unlikely, and if existent, would represent a negligible portion of the overall reef community biomass, and therefore unlikely to provide a significant portion of the overall diet to upper trophic level organisms. We believe this is consistent with comments made by Jon Dodrill and Robert Turpin (see, e.g., Robert Turpin's comments regarding his observance of a very strong inverse relationship between biological utilization and distance from the reefs "exterior"). Based on your comments and those of others to the effect that there may be a need to assign some non-negative percentage of exposure to internal waters, we are amenable to changing this value to some low percentage, if warranted.

Second Round comments:

I believe that we need to put to rest the issue of an "interior (epifaunal) reef community" as quickly as possible. Although I continue to support the approach taken (i.e., unblocking that exposure pathway (Table 2, Cell D10) with a value near zero), my guess is that reasonable people will continue to hold to the belief that epifaunal organisms will utilize interior surfaces of the ship. Robert Turpin's comments not withstanding, we apparently lack the hard evidence to support selection of specific exposure values. I suspect that "professional judgment" will not win the day here, as professionals already seem to be in disagreement (by the way, I recommend that we put to bed the notion that sunlight for photosynthesis is needed to sustain interior organisms -- the determining factor is whether there is sufficient water movement into the ship's interior to transport: a) the pelagic larvae of epifaunal species, and b) organic matter and oxygen to sustain filter feeders). Confounding the issue has been our imprecision in defining the "interior." Is it possible to obtain quantitative information about utilization of reef interiors by epifaunal organisms to support selection of a specific exposure value? If not, we will need to relegate the issue to a discussion of uncertainties.

Response: As discussed in the 6 Jan 05 biology TWG conference call, a compromise position has been achieved that reflects the differing requirements of the human health risk and ecological risk assessments. For purposes of the human health risk assessment, cell D10 (unblocked) will be set as 0% to reflect the consensus opinion that sessile filter feeders in interior ship compartments would represent a very minor/negligible source of PCBs to the higher trophic level organisms consumed by humans. For the ecological risk assessment, exposure to ecological receptor populations will be evaluated by comparing predicted abiotic (bulk water) PCB concentrations to ecological benchmark values.

Dr. Roland Ferry's Comments:

I believe that the approach taken here is both reasonable and defendable. I think that Mark and his team did a nice job breaking out the relevant community compartments and estimating dietary preferences, particularly given the lack of specific information available.

Response: Thank you – comment noted.

I am in full agreement with Wayne's comments regarding documentation.

Response: Comment noted. We have been working to address this in the documentation of the PRAM food web model construct. The documentation issue is clearly one that we need to address and we appreciate the expression of concern.

Regarding the issue of exposures to the interior of the vessel I also believe it needs to be addressed since we are taking it on faith that interior spaces will have higher PCB concentrations and we know that some animals will reside and/or visit interior spaces. I'm not prepared to suggest how important this exposure will be in this case, perhaps not very, but it still remains. I also concur that it should be satisfactorily dealt with using a combination of inserting a value in cell D10 of the model and thoughtful discussion.

Response: The cell for the matrix table (Table 2, Cell D10) is now unshaded to indicate there is a potentially complete (interior) exposure pathway for these organisms. The data users (ecological and human health risk assessors) will use the information provided to make their evaluation for the significance of this pathway.

What follows are some specific suggestions and comments. These are educated guesses, no better than any others and I'm no "expert". If you come by better information or find other scientists who may be more credible, by all means use their suggestions.

Worksheet 1: Water Exposures

As we discussed, myself and others commented on the diel migration of zooplankton suggesting that water exposure of zooplankton should be split more evenly between the epilimnion and hypolimnion. Because planktivores and the piscivores that feed on them will follow the zooplankton (they are heavily preyed upon at night), their exposures should also be split more evenly between the epilimnion and hypolimnion.

Response: We concur. The PRAM will be modified to reflect a 50:50 split for water exposures to the zooplankton community.

Regarding the infaunal or macroinvertebrate community, as I stated, our collections in the northern Gulf show that the community will consist of from some 400-500 species. The majority of theses will be smaller motile invertebrates that move through the sediments. A smaller number of species will be larger bodied animals; some of them free living and some tube dwelling. Tube dwellers often line tubes with materials which may isolate them somewhat from pore water exposure. I can't say what species or groups will likely dominate in any site or sample. In terms of number of species and abundance (individuals) pore water exposure should be primary. In an area where tube dwellers are fairly abundant they may dominate in terms of biomass. In such a case hypolimnion exposure may be primary. If someone has some site specific information (perhaps Rob Turpin) about dominants at the reef site it could help set more reasonable exposure numbers. In lieu of better information one might be safe using a 50-50 split between pore water and hypolimnion.

Response: Comment noted. Since other commenters (e.g., Dr. Johnston) provided a different opinion, we have developed a compromise position that we believe retains a degree of conservatism, as suggested by Dr. Johnston's and your suggestion. We agree that, as the macroinvertebrates employed within the PRAM are represented by burrowing worms , their exposure to pore water would be significant, and probably greater than 50%. However, we think it is unlikely that they would respire 100% pore water. Additionally, it is important to keep in mind that the PRAM is not modeling individual species but rather relevant guilds (i.e., infaunal benthos) such that the assumption that "all" infaunal benthos would respire only sediment pore water is probably inaccurate/unrealistic. Thus our recommendation is that the PRAM configuration should have the infaunal macroinvertebrates respiring 80% sediment pore water and 20% surface water.

Worksheet 2: Dietary Preferences

My main comment here is in regard to the infaunal preference numbers. The infaunal species that are not predacious are generally classified as either deposit or suspension (filter) feeders. Deposit feeders are mainly feeding on the organic matter; zooplankton bodies, fecal pellets (mostly undigested phytoplankton) and detritus from other sources that settle on the seabed. Filter feeders are collecting organic particles from the upper few cm of overlying water. Only a fraction of the total species present ingest actual sediment, usually incidental. Because most of the organic matter consumed for suspension and deposit feeders is derived from algae (microbenthic algae and phytoplankton) and zooplankton, I'd give them about 40-40 with sediment 20%.

Response: Comment noted. Since other commenters (e.g., Dr. Johnston) provided a different opinion, we have attempted to reconcile these opinions. Our current recommendation for the dietary fractions is: 50% sediment, 30% algae, and 20% zooplankton. While the actual dietary fractions of sediment remain high for the benthic macroinvertebrate guilds, it is recognized that there will be direct deposit feeding of algae and zooplankton. The rationale for the selection has been detailed in the PRAM documentation. Key to the consideration is the transfer(s) of PCBs from the sediment itself (representing a PCB" sink) into the detrital food web.

Worksheet 3: Dietary Preference Projections

Planktivores: The progression seems to suggest that as more attached algae become present, it will become a larger % of the planktivore diet. I doubt that, as attached algae will not likely be fed on by this group. I'd spread those %'s among the SS, algae and zooplankton compartments.

Response: The PRAM model construct for the food web, which is specifically designed to trace PCBs within the three communities, has been changed to reflect that the planktivores may not be the most relevant transport pathway for PCBs within the reef community (i.e., not the maximally exposed trophic level II guild). The representative guild selected for the PRAM, based on where maximum exposures concentration would occur, is the omnivorous invertebrate guild that scrapes attached algae and also consumes encrusted filter feeding organisms. The dietary fraction for this guild are 80% attached algae, and 20% encrusted organisms (sessile filter feeders). This is reflected in the revised table and discussed and defended within the PRAM documentation.

Invertebrate forager: In this group I see crabs, urchins, sea slugs, etc., mainly walking and crawling animals, none of which will likely feed much on zooplankton, pelagic planktivores or other organisms free swimming in the water column. My guess is that early on benthic infauna and epifauna will comprise the bulk of the diet and later a larger % of the attached organisms on the vessel.

Response: Comment noted. The diet has been adjusted to reflect a larger percentage of benthic macroinvertebrates. Please refer to the progression shown in the attached table.

The last three groups (foragers and predators) have large initial %'s of their diet coming from benthic epifauna and benthic foragers – just where I'd expect it to come from, although I'd expect infauna to be more important to invertebrate foragers. However, they decrease to smaller %'s and finally go to zero values at day 712. I believe that any food source comprising 50-85% of their initial diet will remain important even as new sources become available. The %'s should decline somewhat, but probably won't go below say 30% of its starting value.

Response: The attempt here was to arrive at the point, at 712 days, where these groups are separated into their respective resident communities. Although the reef vs. benthic *foragers may be comprised of some of the same species, they are separated into distinct populations, those resident over the sediment or those on the reef once the reef has become fully established. This is described more completely in the final documentation along with the rationale, which is associated with maximizing exposure and evaluating relative risks between communities.*

Dr. Jon Dodrill's Comments:

1) We appreciate the effort that Mark, Bob and others have made to expand the trophic levels as well as feeding guilds within the categories. This expanded food web, though more difficult to incorporate into the model, I believe represents a more defensible approach than a simplistic food chain.

Response: Thank you – comment noted.

2) By choosing to be generic in each of your categories (example, Benthic Forager (TL-III_; Reef Predator (TL-IV)), but then assigning specific percentages for various food items consumed by the "generic" organisms, you have entered the realm of intuition, gestalt, or educated guessing. We all recognize that the pulse modeling sheet is the most subjective and probably the least defensible. I personally probably could not defend the reasons why these specific percentages were selected although I accept the fact that most seem intuitively reasonable. If someone were to ask me why at day 712 there are no pelagic planktivores in the reef predator's diet, I would be very hard pressed to defend that assessment.

Response: We agree that any of the specific percentages are subjective and would be difficult to defend, given the paucity of information available regarding diet progression as an artificial reef develops. But it is intuitively clear that a diet progression must take place as reef organisms colonize the reef and communities are established. The proposed percentages simply represent an orderly progression of diet, as reef forage becomes available over time.

With respect to your comment regarding reef predator diet, and the possibility that some individual reef predator might someday consume a pelagic planktivore: yes, that is certainly a possibility. However, for modeling purposes one needs to characterize groups with common dietary characteristics such that the diets, and exposures associated with the diets, are representative of that guild. Hence, by definition, reef predators predominately eat reef-associated fish and not pelagic fish. Whereas, by definition, in the pelagic community, pelagic predators predominately eat pelagic fish. While mixing diets from the three communities may be a useful exercise in evaluating a specific fish species, it is not consistent with the goal of evaluating the potential exposure to a specific guild as a whole. It should be noted that the generic reef predator, as modeled in PRAM, will provide a more conservative estimate of potential PCB biouptake than a species, such as gag grouper, which also feeds on pelagic planktivores.

For the Oriskany, we expect a dominant reef predator will be the gag grouper. Gag grouper feed heavily on schooling pelagic planktivores (scad, herring) when these planktivores are at artificial reef sites by the thousands, sometimes within days after a vessel is deployed

Response: We recognize that the gag grouper is a species of particular interest, and that this species does not readily fit into the strict definition of a reef predator. Rather, we would place it in the pelagic predator guild, since its diet is primarily pelagic fish, and discuss the fact that gag grouper have a mixed diet.

Dr. William Lindberg (University of Florida) reported that as much as 80 percent of the gag's diet during the summer off the Florida Big Bend are schooling planktivores and they pick them off in the water column. When, during winter, these planktivores leave, the gag's diet in the Florida Big Bend shifts to tomtate grunts, black sea bass, etc. So to say at year one or two that a reef predator does not feed on any pelagic planktivores is probably not defensible when one of the primary vertebrate reef predators expected on the Oriskany probably will still be feeding at least seasonally on pelagic planktivores. Similarly can we defend the example of a invertebrate forager feeding on a pelagic planktivore 15% of the time on day 1 and 10% on day 34? Again I personally couldn't. Does anyone have an example? Are we envisioning such invertebrate as Florida lobsters or slipper lobsters feeding on dead pelagic planktivores falling out of the water column because neither they nor a common octopus for example are going to be swimming up into the water column? Are you suggesting squid, yet squid wouldn't have as 35% of its diet attached algae. <u>All I am saying, is, if one PRAM model objective is defensibility then you need to be ready to have some concrete examples relatable to this Oriskany project that at least fall somewhere in these dietary preference percentages proposed for these generic trophic levels.</u> We need to be prepared to have a specific example(s) of real world organisms for each trophic level for which there is data to show that its dietary preferences as reported in the literature at least fall within the realm of common sense acceptability as relates to the percentages shown in these tables. I don't think "Professional Judgment by Consensus" trumps being able to have on hand (or better yet in the writeup) some specific references that at least support some of these very specific percents that are laid out here. –

Response: Comments noted. In the PRAM write-up and the SHHRA we will discuss guilds with specific examples and relate them to the dietary preferences proposed for the generic trophic levels; where appropriate, we will discuss variances that may be significant in the context of characterizing representative species' exposures.

3) What do these % dietary preferences represent: are they volumetric, by % weight, % number of prey organisms?

Response: The percentage dietary preferences are related to the energy budgets in PRAM. That is, the important parameter is that the various percentages add up to 100% of the caloric intake for the organism. The percentages are based on a caloric content basis, where if 10% of the diet is zooplankton, based on the total caloric consumption of the predator, 10% of the animal's daily caloric intake comes from zooplankton. The mass of zooplankton consumed by the predator is based on the caloric content of the zooplankton and assimilation efficiency of zooplankton calories by the predator.

4) Overall I agree with Roland Ferry's comments submitted.

Response: Comment noted. Please see responses to Dr. Ferry's comments.

5) I support the concept of utilizing a very conservative approach. However, intuitively I don't believe that the carrier will function as a theoretical framework of "cheesecloth" with respect to transport of PCBs. If that were the case, the U.S.S. Arizona, on the bottom in Pearl Harbor, now 63 years later, still wouldn't have 500,000 gallons of fuel on board, with only a fraction of it leaking out. The leaking may be a steady state rate, but unless that ship is pumped, someday there will be a much greater pulse of released oil.

In the Oriskany, I believe elevated levels of PCBs will build up in some of those hundreds of compartments on the Oriskany at lower levels below the flight deck where PCB containing bulkhead insulation and electrical cable remain. Personally, I don't see the ultimate steady state release achieved for the life of the wreck by year two.

At some point when there is a catastrophic hull failure (probably more than a half century from now) and interior water circulation abruptly increases there will be increased water movement with elevated PCB concentrations. If this hull is expected to behave like Swiss cheese, why did they have to run ventilation hoses down into the interior of the ship and check the air chemistry if there was steady air circulation?. Why would one expect to see unimpeded water circulation throughout the ship?. This is not a ship which to my knowledge is going to have gaping holes cut in the side (as was the case of the Yukon and other small Canadian DE's sunk as artificial reefs). The opened sea chests will be effectively sealed off again once the hull digs into the bottom immediately upon sinking. In short, I think you'll have a steady state situation in two years with the island, the hanger deck and the mezzanine deck and perhaps for some years thereafter for the ship as a whole as with the leaky oil Arizona.. But one day there will be some sort of storm induced catastrophic hull failure as has occurred with the smaller navy vessels on the east coast (though Oriskany hull integrity will fail at a much later date) and there will be another PCB pulse. I think you will need to address this issue in the write up in justifying your methodology.

Response: Comments noted. We agree that modeling the vessel as "porous" is an artificial construct. We believe that it is a conservative approach to assume that the ship will leach PCBs continuously (i.e., with an assumption that there will be no PCB mass depletion over time), and that significant PCB releases into the environment will occur from the moment that the vessel is deployed on the sea floor (i.e. all PCB-containing solid materials will begin releasing PCBs right away, and there will be no barriers to the PCBs coming under the influence of an assumed internal water current which will facilitate transport of the PCBs to an external environment). We believe this is a conservative assumption from the standpoint of assessing exposure to the occupants of the reef. (Conversely, if an assumption were made that most of the PCBs would remain internal to the ship for many years, and not be released to the external environment, then the corollary would be that the reef occupants would only be exposed to very low levels of PCBs in the abiotic and biotic media for many years.)

Regarding the concern that PCBs could build up in internal, essentially sealed off compartments of the ship, and be released via a catastrophic failure: we have modeled this scenario in the context of SINKEX (although this document was not provided to EPA for review). What we found in that evaluation was that a single, large "pulse" release of PCBs into the environment did not equate to a significant human health risk, with respect to risk associated with human ingestion of fish. The analysis revealed that catastrophic release actually reduced the ultimate fish tissue concentrations in top predators as the PCBs were advected away from the vessel too quickly for the system to adsorb them. A slow constant release, because of the slow dynamics associated with the accumulation and trophic transfers of PCBs, will result in higher concentrations.

Regarding the comment that it may take longer than two years to reach a steady-state leach rate and/or steady-state condition in the reef: The "constant" PCB (homolog-specific) leach rates used in PRAM were based on the leachate studies conducted by SSC-SD. In these experiments, specific materials were immersed in sea water, and the leach rates recorded as a function of time in immersion. After initial periods where the leach rates increased to a maximum (taking days or weeks), the leach rates decreased over time, reaching or approaching an asymptotic value. These curves were used to derive an appropriate "steady-state" or "constant" leach rate for each PCB homolog group. The experimental period was approximately two years. By that time, all homolog rates had reached or approached asymptotic values. With regard to the two-period period assumed in PRAM (to reach a steady-state condition), this was based on an assumption that it would take several months, to more than a year, for the reef to mature into a viable reef, where all the occupants of the reef would be present. The rationale for the two year time frame is associated with the development of a complete and functional food web for the reef.

6) The model has to be able to be communicated to and made understandable and defensible to the non modeler, who nevertheless still has some common sense.

Response: We appreciate your comments, and will strive to make the description of the model understandable and defensible.

7) I agree with Robert Turpin, that one will never see reef fish or foraging macroinvertebrates in the labyrinth of compartments and passageways in the lower levels of this ship in complete darkness, with little or no current activity. Bacterial colonies probably. Time spent by a school of red snapper technically inside the ship on the bridge just inside where all the windows have been removed along with most of the bulkhead insulation and the wire cable would present a different interior exposure scenario than these lower level compartments with all bulkhead insulation and all wiring remaining. However, I do understand the modeling challenges Mark has to deal with and that certain assumptions have to be made. They just need to be pointed out and explained.

Response: We concur with your comments. Thank you for your appreciation of the challenges.

CAPT Robert Turpin's comments:

It is my understanding that the "communities" in the trophic matrix represent a summation of exposure. For example, if all the organisms are exposed for 50% of the time, OR if 50% of the organisms are exposed 100% of the time, the resultant should be the same. If I misunderstand, please correct me. However, if I am correct, then it is most appropriate and representative to assign some small percentage of the reef epifauna to interior water exposure.

Response: We agree that, in the general sense, such trade-offs can be made, so long as the values are clearly explained and understood by all. Please note our responses to Wayne Munns' comments above.

From thousands of dives, many on artificial reefs, many of which my sole purpose was extracting fish and invertebrates for scientific and/or culinary objectives, I have observed a very strong inverse relationship between biological utilization and distance from the reefs "exterior". My videography should be sufficient to demonstrate, but will be more than happy to collect samples, better yet accompany anyone to any of my underwater vessels that feels the need to verify. It is my strong preference that we do not invent a community to satisfy the need to accurately model the small percentage of epifauna that will inhabit the "first" interior compartments. When viewing the ship from a volumetric perspective (and I think the "Virtual Oriskany" model can do this), it should be easy to calculate and compare the volumes of the "true" interior of the ship as well as the "inside of the outside" (that first compartment that can sustain life (food and dissolved oxygen; light for the photosynthetic organisms).

Response: We appreciate your knowledge and experience with regards to reef habitat, and defer to your knowledge with respect to observing that a very strong inverse relationship exists between biological utilization and distance from the reefs "exterior".

Second Round Comments:

Table 1

1) Title of the 4th column should be changed (from "sediment") to Detritus or POM (Particulate Organic Matter) to identify the materials that contain biological energy.

Response: As discussed in the 6 Jan 05 biology TWG conference call, the term "sediment" refers to any material within the sediment bed that supplies the biological energy input. The column header will be footnoted to indicate that detritus or POM is the primary source of this energy input.

2) Title of 5th column should be changed from Algae to Phytoplankton.

Response: We agree that the term "phytoplankton" more accurately describes the primary producer (algal) population in the water column. The requested change will be made.

3) Reef "Vertebrate Predator (TL-IV)" and Reef "Vertebrate Forager (TL-III)" diets should reflect some percentage of energy taken from the surrounding benthos. This is clearly represented by many papers on reef trophodynamics. As we agreed on Conf. Call, a value of 25% (spread across Infaunal Benthos & Epifaunal Benthos for Vert. Forager; spread across Infaunal Benthos, Epifaunal Benthos, and Benthic Forager for Reef Predator). Reductions of other columns should be proportional.

Response: As discussed in the 6 Jan 05 biology TWG conference call, because of the opportunistic nature of their feeding behaviors, Vertebrate Reef Predators (TL-IV) and Vertebrate Reef Foragers (TL-III) undoubtedly obtain a significant portion of their diet from the benthic community. The Vertebrate Reef Forager (TL-III) and Vertebrate Reef Predator (TL-IV) food intake values in Table 1 will be revised as suggested.

4) (For the record) I think that sessile filter feeders would consume a ratio of phyto-:zoo-plankton more evenly than 80:20.

Response: Response noted. As discussed in the 6 Jan 05 biology TWG, the proposed dietary breakdown is intended to demonstrate PCB tracing through the food web, whereby sessile filter feeders derive a greater portion of their dietary PCB from ingestion of trophic level I (phytoplankton) organisms than trophic level II (zooplankton).

Table 2

1) Water exposure of Reef/Vessel sessile filter feeder will be exposed to some small (i.e., 0-5%) percentage of interior water.

Response: Agreed. As discussed previously, cell D10 of the model (interior water exposure to sessile filter feeders) has been unblocked to allow the user to input site-specific values, as appropriate. For evaluating potential human health risks, this value will be set at 0%, as this pathway is thought to represent a negligible proportion of the overall PCB uptake into upper trophic level organisms likely to be consumed by humans.

Table 3

Changes should reflect the changes in values accepted for Table 1. As we discussed on conf. Call, those changes may be reflected from 180 days and "later".

Response: Agreed. Changes to the diet for Vertebrate Reef Foragers (TL-III) have been modified for the three time periods in question (days 180, 360, and 720) as discussed above for Table 1. The Vertebrate Reef Predator (TL-IV) was modified for day 720, as discussed above for Table 1. The diet for the Vertebrate Reef Predator (TL-IV) was not modified for days 180 and 360, as these days already reflect a high proportion of the overall diet originating from the benthos (50% at day 360; 60% at day 180).

Turbulence created by placement of Oriskany on the sea floor will mix waters surrounding the reef. As shown in the diagram from Seaman & Sprague (Fig. 4.13), reef occupancy of 20% of water depth will create height of turbulence nearly 100% of water column. Excluding superstructure, Oriskany (from keel to flight deck) will occupy nearly 40% of water column. Turbulence will be <u>very</u> nearly 100% f water column.

Also, Thermocline depth estimate I provided in Atlanta (Nov '04) was not intended to indicate Δ T/S (temp/salinity) magnitude of a true "pycnocline". Summer thermoclines are eliminated in winter by convective mixing. A variable "reverse" – thermocline may occur during cold weather events. Shallow continental shelf waters are more highly mixed than the model represents. That being said, I support the consensus of the TWG regarding the conservatism provided by assuming upper & lower water masses.

Response: We appreciate the insight you have provided regarding turbulent mixing, and the likelihood that turbulence/vertical mixing associated with the ORISKANY will probably disrupt any thermocline overlying the reef. As discussed in the 6 Jan 05 biology TWG, the approach currently used by PRAM assumes that a thermocline exists, and that advective/turbulent mixing does not occur above the thermocline. This is a conservative approach that is likely to overestimate PCB uptake into some organisms. Because of the very tight timeframe we are currently committed to, we will not be able to revise PRAM to reflect turbulent mixing throughout the entire water column prior to the next submittal of the model. We will reserve the option to incorporate the more realistic mixing pattern you have identified into future versions of PRAM.

Overall, I am pleased with the products of everyone's hard work. I think we have constructed a good model, and I look forward to seeing the results. Thanks to all for the dedication to a job well done!

Response: We appreciate the support of the TWG for arriving at consensus on numerous difficult technical issues necessary for successful completion of the project. We believe the hard work of a number of individuals, particularly the author of the model, Mark Goodrich, will result in a quality product we can all be proud of.

<u>Dr. Robert Johnston's Comments</u>:

Benthic community:

The benthic community is composed of organisms living in or on the bottom (US EPA 2004). The benthic community represented in the PRAM includes the benthic infauna, benthic epifauna, benthic foragers, and benthic predators. The modeled infauna are representative of macrobenthic suspension feeders, deposit feeders, and benthic carnivores that spend a predominant portion of their life living within the sediments. Examples of benthic infauna include nematodes, worms, , and a few amphipods, etc. While recognizing that a large portion of the benthic infauna population is made up of micro-organisms (organisms smaller than 0.5 mm, Novitsky 1983) PRAM does not explicitly model the microbial community, but considers the contribution of the microbial community as organic matter or detrital material, which is a major dietary component modeled within the PRAM for the benthic infauna (see below).

Response: Other commenters (e.g., Dr. Ferry) have recommended that a lower sediment dietary fraction be used. We have developed a compromise between your suggestion and his, which is present in the revised table and defended within the PRAM documentation.

The benthic infauna compartment is composed of the biologically active zone of the sediment, the interstitial water (pore water). The overlying water just above (2-6 cm) represents the sediment-water interface through which PCBs are transported to and from the sediment bed. The pore water and this overlying boundary layer water are modeled within the PRAM because they are geochemically distinct from the waters below the pycnocline (thermocline). The overlying water contains higher amounts of sedimentary flocs, organic matter, and suspended particles than is present in the water column, and any near-bottom currents present in the water column would be strongly dampened by friction with the bottom at the sediment water interface. Toxicological studies have shown that overlying waters are similar to interstitial water with respect to partitioning and toxicity (Berry et al. 2003a, b). To reflect these processes PRAM uses 100% pore water to model water exposure to benthic infauna (Table "water-exposure").

Response: We do not agree that 100% pore water exposure is appropriate. Please see our response to Dr. Ferry's comment regarding pore water exposures.

Note that portions of Dr Johnston's comments were provided as embedded text statements. We hope that this will not be confusing to other reviewers. (The embedded text statements are shown in highlight in this response document.)

The benthic infauna diet is composed of 85% sediment, 10% algae, and 20% zooplankton (Table "diet Pel & Ben"). It should be noted that the benthic infauna are not really consuming sediment, rather they are consuming the organic matter (e.g., microfauna) present on the particles, the inorganic matter would pass through the gut, so dietary requirements take into account the amount of calories associated with the organic matter that must be consumed and the energy requirements for the organism(i.e., grams/day consumed is organic matter, not just bulk sediment, OM ~= 2*TOC).

Response: We are in agreement that consumption is based on the caloric content of the sediment detrital fraction.

The benthic epifauna community is the organisms that live on the bottom, but spend their time predominantly above the sediment-water interface. Examples of benthic epifauna are sea slugs, sea urchins, sea anemones, shrimp, mussels, etc. Because of their close association with the bottom sediments PRAM assumes that water exposure is 50% pore water and 50% below pycnocline water (Table "water-exposure"). The benthic infauna diet consists of 50% sediment organic matter, 15% organic matter on suspended solids (i.e. detritus), 10% algae, and 10% zooplankton (Table "diet Pel & Ben").

Response: The diet for the benthic infaunal macroinvertebrates has been adjusted to account for the differences in opinions between commenters and is discussed within the PRAM documentation. Please see our responses to Dr. Ferry's comments.

The benthic foragers are the lobsters, sea stars, crabs, octopus, etc., that feed on the infauna (50%) and epibenthic community (45%) (Table "diet Pel & Ben"). Because the benthic foragers feed on infauna, PRAM also models incidental consumption of sediment organic matter by assuming that incidental sediment consumption of benthic foragers is 10% of the epifaunal benthos consumed (rounded to 5%). This assumption is consistent with other risk assessments that have evaluated exposure from incidental sediment exposure as part of the consumption pathway (URS 1996, MESO 2000). Water exposure to benthic foragers is modeled as 75% below pycnocline water and 25% pore water (Table "water-exposure"), reflecting the relatively greater mobility of benthic foragers and the less time that they are actually in contact with bedded sediments.

Response: We have adjusted the diets and water exposures to the benthos in recognition of your and Dr. Ferry's comments, and have developed a written rationale for the values recommended in the attached table.

The top predators in the benthic community are the flat fish, skates, toad fish, eels, and other carnivorous fish that feed on the benthic foragers (58%), epifauna (20%), and infauna (20%) (Table "diet Pel & Ben"). Because the benthic predators also feed on infauna, incidental sediment consumption was set to 10% of the epifaunal benthos consumed (2%). Because most of the benthic predators spend most of their time in the water column rather than in the sediment, water exposure is modeled as 90% below pycnocline water and 10% pore water (Table "water-exposure")".

Response: We have adjusted the diets and water exposures to the benthos in recognition of your and Dr. Ferry's comments, and have developed a written rationale for the values recommended in the attached table.

APPENDIX H

EXAMPLE PRAM OUTPUT

ZOI = 2

PCB MODELING RESULTS - PROSPECTIVE RISK EVALUATION

RISK ESTIMATES FOR Ex-Oriskany CV34

	Cancer Risk Adult & Child		Hazard Adult & Child		Cancer Risk Child		Hazard Child	
RISK ESTIMATES	RME	CTE	RME	CTE	RME	CTE	RME	CTE
Benthic fish (flounder)	7.29E-08	5.64E-09	4.25E-03	9.75E-04	2.14E-08	4.34E-09	6.24E-03	1.12E-03
Benthic shellfish (lobster)	2.12E-08	1.64E-09	1.24E-03	2.84E-04	6.22E-09	1.26E-09	1.81E-03	3.27E-04
Pelagic fish (jack)	3.57E-08	2.77E-09	2.08E-03	4.78E-04	1.05E-08	2.13E-09	3.06E-03	5.51E-04
Reef fish TL-IV (grouper)	6.94E-06	5.37E-07	4.05E-01	9.29E-02	2.04E-06	4.13E-07	5.94E-01	1.07E-01
Reef fish TL-III (triggerfish)	4.03E-06	3.12E-07	2.35E-01	5.39E-02	1.18E-06	2.40E-07	3.45E-01	6.22E-02
Reef shellfish (crab)	2.23E-06	1.73E-07	1.30E-01	2.98E-02	6.54E-07	1.33E-07	1.91E-01	3.44E-02

PREDICTED EXPOSURE CONCENTRATIONS (mg/kg in fresh weight)	
Benthic fish (flounder)	1.18E-03
Benthic shellfish (lobster)	3.45E-04
Pelagic fish (jack)	5.80E-04
Reef fish TL-IV (grouper)	1.13E-01
Reef fish TL-III (triggerfish)	6.55E-02
Reef shellfish (crab)	3.62E-02

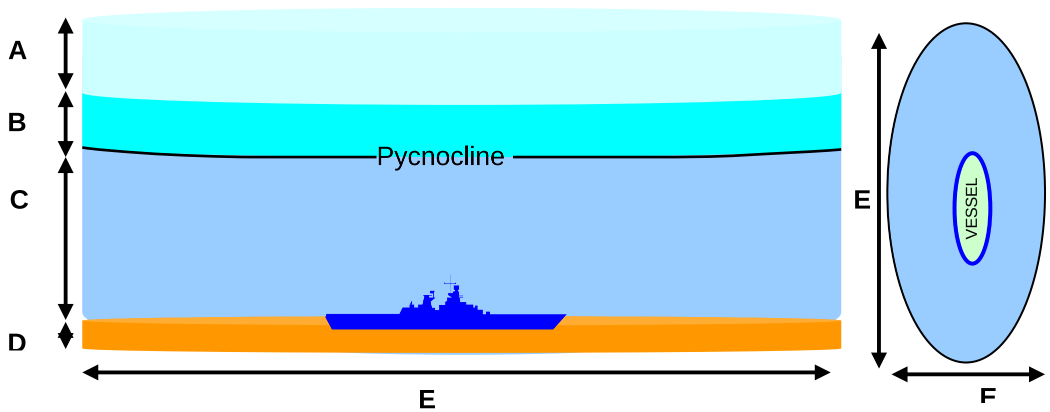
RISK INPUTS - Adult	RME	CTE
Body Weight (BWa) (kg)	70	70
Exposure Frequency (EFa) (days)	365	365
Exposure Duration (EDa) (years)	24	3
Ingestion Rate (IRa) (kg/day)	0.0261	0.0072
Averaging Time for cancer (ATc)	25550	25550
Averaging Time for noncancer (ATnc-adult)	8760	1095
Slope Factor (mg/kg-day)	2	1
Reference dose for PCBs (RfD) (mg/kg-day)	2.00E-05	4.50E-05
Fractional Ingestion factor (FI)	0.17	0.25
Ingestion Rates Based on Data from	Gulf Coast	

RISK INPUTS - Child	RME	CTE
Body Weight (BWc) (kg)	15	15
Exposure Frequency (EFc) (days)	365	365
Exposure Duration (EDc) (years)	6	6
Ingestion Rate (IRc) (kg/day)	0.0092916	0.0025632
Averaging Time for cancer (ATc)	25550	25550
Averaging Time for noncancer (ATnc-child)	2190	2190
Slope Factor (mg/kg-day)	2	1
Reference dose for PCBs (RfD) (mg/kg-day)	2.00E-05	4.50E-05
Fractional Ingestion factor (FI)	0.17	0.25
Child - Adult IR scaling factor	0.356	

Zone of Influence Multiplier	2
Scenario run on	5/11/05 13:36

PCB-LADEN MATERIAL INPUTS	Fraction PCB	Release Rate (ng/g-d)	kg Material Onboard	PCB Release (ng/day)
Ventilation Gaskets	3.14E-05	1.58E+03	1.46E+03	7.23E+04
Lubricants	1.03E-04	2.20E+03	0.00E+00	0.00E+00
Foam Rubber Material	7.60E-03	2.62E+00	0.00E+00	0.00E+00
Black Rubber Material	5.29E-05	1.58E+03	5.40E+03	4.50E+05
Electrical Cable	1.85E-03	2.79E+02	2.96E+05	1.53E+08
Bulkhead Insulation Material	5.37E-04	6.76E+04	1.44E+04	5.22E+08
Aluminum Paint	2.00E-05	1.11E+04	3.87E+05	8.62E+07
Total				7.62E+08

Ex-Oriskany CV34	
Displacement (tons)	27100
Length (ft)	888
Beam (ft)	120



ZOI =	2	
Spatial Footprint on Ocean Floor		
	1.56E+04	m2
	6.00E-03	mile2
Modeled Dimensions Outside the Vessel		
A	1.00E+01	m
B	1.50E+01	m
C	5.00E+01	m
D	1.00E-01	m
E	3.00E+02	m
F	6.60E+01	m
Volumes		
Air Column		
Air	1.56E+05	m3
Upper Water Column		
Water	2.33E+05	m3
TSS	1.56E+00	m3
Lower Water Column		
Water	7.24E+05	m3
TSS	4.82E+00	m3
Inside Vessel		
Water	5.38E+04	m3
TSS	3.59E-01	m3
Sediment Bed		
Sediment	7.78E+02	m3

Abiotic Inputs

Air Column

Active air space height above water column (m)	10

Total PCB concentrations

Air Column

Air	6.68E-17	g/m3

Air current (m/h)	13677
Upper Water Column	
Temperature (°C)	24.5
Water depth (m)	15
Total suspended solids (mg/L)	10
Dissolved organic carbon (mg/L)	0.6
Dissolved oxygen (mg/L)	6.12
Lower Water Column	
Temperature (°C)	19.5
Water depth (m)	50
Total suspended solids (mg/L)	10
Dissolved organic carbon (mg/L)	0.6
Dissolved oxygen (mg/L)	4.59
Inside Vessel	
Temperature (°C)	19.5
Total suspended solids (mg/L)	10
Dissolved organic carbon (mg/L)	0.6
Dissolved oxygen (mg/L)	4.59
Sediment Bed	
Sediment density (g/cm3)	1.5
Active sediment depth (m)	0.1
Sediment fraction organic carbon	0.01
All Regions	
Suspended solids density (g/cm3)	1.5
Suspended solids fraction organic carbon	0.15
Dissolved organic carbon density (g/cm3)	1
Water current - to out of the ZOI (m/h)	926
Water current - inside to outside the vessel (m/h)	9.26

Upper Water Column		
Freely dissolved in water	1.02E-12	mg/L
Suspended solids	1.33E-08	mg/kg
Dissolved organic carbon	1.78E-07	mg/kg
Lower Water Column		
Freely dissolved in water	4.39E-09	mg/L
Suspended solids	1.08E-04	mg/kg
Dissolved organic carbon	9.88E-04	mg/kg
Inside Vessel		
Freely dissolved in water	1.80E-06	mg/L
Suspended solids	4.44E-02	mg/kg
Dissolved organic carbon	4.06E-01	mg/kg
Sediment Bed		
Freely dissolved in pore water	4.39E-09	mg/L
Bedded sediment	7.19E-06	mg/kg
Dissolved organic carbon in pore water	9.88E-04	mg/kg

Total PCB concentrations in biota			**Percent Exposures**	
Pelagic Community			Upper WC	Lower WC
Phytoplankton (TL-I)	1.67E-09	mg/kg	100%	0%
Zooplankton (TL-II)	7.72E-05	mg/kg	50%	50%
Planktivore (TL-III)	3.74E-04	mg/kg	80%	20%
Piscivore (TL-IV)	5.80E-04	mg/kg	80%	20%
Reef / Vessel Community			Lower WC	Vessel Int.
Attached Algae (TL-I)	7.23E-06	mg/kg	100%	0%
Sessile filter feeder (TL-II)	1.58E-04	mg/kg	100%	0%
Invertebrate Omnivore (TL-II)	1.69E-02	mg/kg	80%	20%
Invertebrate Forager (TL-III)	3.62E-02	mg/kg	70%	30%
Vertebrate Forager (TL-III)	6.55E-02	mg/kg	70%	30%
Predator (TL-IV)	1.13E-01	mg/kg	80%	20%
Benthic Community			Lower WC	Pore Water
Infaunal invert. (TL-II)	5.48E-05	mg/kg	20%	80%
Epifaunal invert. (TL-II)	1.51E-04	mg/kg	50%	50%
Forager (TL-III)	3.45E-04	mg/kg	75%	25%
Predator (TL-IV)	1.18E-03	mg/kg	90%	10%

PCB MODELING RESULTS - PROSPECTIVE RISK EVALUATION
RISK ESTIMATES FOR Ex-Oriskany CV34 High-End Weight of PCB-Laden Materials
Supplemental Information

Scenario Run on 10/21/2004 14:10

PCB Homolog	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Molecular Weight (g/mol)	1.89E+02	2.23E+02	2.58E+02	2.92E+02	3.26E+02	3.61E+02	3.95E+02	4.30E+02	4.64E+02	4.99E+02
Solubility (mg/L)	2.91E+00	6.78E-01	8.14E-02	6.67E-02	2.61E-02	9.50E-04	2.30E-04	2.11E-08	4.02E-09	1.69E-10
Solubility (mol/m^3)	1.54E-02	3.04E-03	3.16E-04	2.28E-04	8.00E-05	2.63E-06	5.82E-07	4.91E-11	8.65E-12	3.38E-13
Vapor Pressure (Pa)	6.32E-01	1.41E-01	5.11E-02	2.08E-02	2.96E-03	3.43E-03	2.56E-04	8.65E-05	2.77E-05	1.41E-05
Henry's (Pa-m^3/mol)	4.10E+01	4.65E+01	1.62E+02	9.10E+01	3.70E+01	1.30E+03	4.40E+02	1.76E+06	3.20E+06	4.18E+07
$\log_{10}K_{ow}$ =	4.47	5.24	5.52	5.92	6.50	6.98	7.19	7.70	8.35	9.60
$\log_{10}K_{oc}$ =	3.66	4.06	4.63	4.65	4.94	6.08	6.34	6.46	6.97	7.94
$\log_{10}K_{doc}$ =	3.34	4.11	4.39	4.79	5.51	5.85	6.06	6.57	7.22	8.47
Chemical emission rate (g/day)	1.37E-05	1.12E-01	9.95E-03	1.69E-01	3.20E-01	7.57E-02	7.37E-02	0.00E+00	8.28E-04	4.62E-04
Chemical emission rate (mol/hr)	3.03E-09	2.09E-05	1.61E-06	2.42E-05	4.08E-05	8.74E-06	7.77E-06	0.00E+00	7.43E-08	3.86E-08
Biodegradation in sediment (1/hr)	0	0	0	0	0	0	0	0	0	0
Biodegradation in water (1/hr)	0	0	0	0	0	0	0	0	0	0

	Ventilation Gaskets	Lubricants	Foam Rubber Material	Black Rubber Material	Electrical Cable	Bulkhead Insulation Material	Aluminized Paint
Fraction PCB in Material (wt/wt)	0.0000314	0.000103	0.76%	0.0000529	0.00185	0.000537	0.00002
Material Mass Onboard (kg)	1459	0	0	5397	296419	14379	386528
Total PCBs (kg)	0.0458126	0	0	0.2855013	548.37515	7.721523	7.73056
Total PCB Release rate (ng/g-PCB per day)	1.58E+03	2.20E+03	2.62E+00	1.58E+03	2.79E+02	6.76E+04	1.11E+04

Release Rates in nanograms PCB per gram of PCB within the Material	Ventilation Gaskets	Lubricants	Foam Rubber Material	Black Rubber Material	Electrical Cable	Bulkhead Insulation Material	Aluminized Paint
Monochlorobiphenyl	4.14E+01	3.47E+01	0.00E+00	4.14E+01	0.00E+00	0.00E+00	0.00E+00
Dichlorobiphenyl	1.27E+03	1.72E+02	3.08E-02	1.27E+03	2.03E+02	5.36E+00	0.00E+00
Trichlorobiphenyl	5.66E+01	8.97E+01	7.63E-02	5.66E+01	1.14E+00	9.44E+02	2.61E+02
Tetrachlorobiphenyl	1.44E+02	1.08E+03	1.29E+00	1.44E+02	1.57E+01	2.07E+04	1.23E+02
Pentachlorobiphenyl	6.31E+01	6.60E+02	3.90E-02	6.31E+01	1.80E+01	3.79E+04	2.24E+03
Hexachlorobiphenyl	0.00E+00	9.42E+01	5.34E-01	0.00E+00	2.41E+01	6.76E+03	1.33E+03
Heptachlorobiphenyl	5.04E+00	7.17E+01	6.46E-01	5.04E+00	1.47E+01	1.30E+03	7.19E+03
Octachlorobiphenyl	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Nonachlorobiphenyl	0.00E+00	0.00E+00	1.72E-03	0.00E+00	1.51E+00	0.00E+00	0.00E+00
Decachlorobiphenyl	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.43E-01	0.00E+00	0.00E+00
Total	**1.58E+03**	**2.20E+03**	**2.62E+00**	**1.58E+03**	**2.79E+02**	**6.76E+04**	**1.11E+04**

Release Rates in nanograms PCB per Day	Ventilation Gaskets	Lubricants	Foam Rubber Material	Black Rubber Material	Electrical Cable	Bulkhead Insulation Material	Aluminized Paint	Total
Monochlorobiphenyl	1.90E+03	0.00E+00	0.00E+00	1.18E+04	0.00E+00	0.00E+00	0.00E+00	1.37E+04
Dichlorobiphenyl	5.80E+04	0.00E+00	0.00E+00	3.62E+05	1.11E+08	4.14E+04	0.00E+00	1.12E+08
Trichlorobiphenyl	2.59E+03	0.00E+00	0.00E+00	1.62E+04	6.25E+05	7.29E+06	2.02E+06	9.95E+06
Tetrachlorobiphenyl	6.60E+03	0.00E+00	0.00E+00	4.11E+04	8.61E+06	1.60E+08	9.51E+05	1.69E+08
Pentachlorobiphenyl	2.89E+03	0.00E+00	0.00E+00	1.80E+04	9.87E+06	2.93E+08	1.73E+07	3.20E+08
Hexachlorobiphenyl	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.32E+07	5.22E+07	1.03E+07	7.57E+07
Heptachlorobiphenyl	2.31E+02	0.00E+00	0.00E+00	1.44E+03	8.06E+06	1.01E+07	5.56E+07	7.37E+07
Octachlorobiphenyl	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Nonachlorobiphenyl	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.28E+05	0.00E+00	0.00E+00	8.28E+05
Decachlorobiphenyl	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.62E+05	0.00E+00	0.00E+00	4.62E+05
Total	7.23E+04	0.00E+00	0.00E+00	4.50E+05	1.53E+08	5.22E+08	8.62E+07	7.62E+08

PCB MODELING RESULTS - PROSPECTIVE RISK EVALUATION
RISK ESTIMATES FOR Ex-Oriskany CV34 High-End Weight of PCB-Laden Materials
Supplemental Information

Air	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Fugacity (Pa)	3.22E-20	1.98E-16	1.30E-17	1.74E-16	1.91E-16	6.72E-18	2.40E-18	0.00E+00	8.51E-22	2.74E-24
Air concentration (g/m3)	2.47E-21	1.80E-17	1.37E-18	2.07E-17	2.54E-17	9.88E-19	3.86E-19	0.00E+00	1.61E-22	5.56E-25

Upper Water Column	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Fugacity (Pa)	6.67E-18	5.04E-14	1.22E-14	9.85E-14	4.71E-14	5.99E-14	7.57E-15	0.00E+00	2.11E-14	9.20E-16
Water concentration (mg/L)	3.07E-17	2.42E-13	1.95E-14	3.16E-13	4.15E-13	1.66E-14	6.80E-15	0.00E+00	3.06E-18	1.10E-20
Suspended solids concentration (mg/kg)	2.12E-14	4.15E-10	1.23E-10	2.14E-09	5.36E-09	2.99E-09	2.23E-09	0.00E+00	4.24E-12	1.44E-13
Dissolved organic carbon (mg/kg)	6.77E-14	3.09E-09	4.79E-10	1.95E-08	1.35E-07	1.16E-08	7.79E-09	0.00E+00	5.09E-11	3.25E-12

Lower Water Column	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Fugacity (Pa)	2.35E-14	1.81E-10	4.61E-11	3.80E-10	2.18E-10	6.75E-10	1.31E-10	0.00E+00	1.83E-09	9.95E-10
Water concentration (mg/L)	1.08E-13	8.67E-10	7.34E-11	1.22E-09	1.92E-09	1.87E-10	1.18E-10	0.00E+00	2.65E-13	1.19E-14
Suspended solids concentration (mg/kg)	7.47E-11	1.48E-06	4.64E-07	8.25E-06	2.48E-05	3.37E-05	3.87E-05	0.00E+00	3.68E-07	1.55E-07
Dissolved organic carbon (mg/kg)	2.38E-10	1.11E-05	1.80E-06	7.54E-05	6.26E-04	1.31E-04	1.35E-04	0.00E+00	4.41E-06	3.52E-06

Inside the Vessel	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Fugacity (Pa)	9.67E-12	7.43E-08	1.89E-08	1.56E-07	8.96E-08	2.77E-07	5.40E-08	0.00E+00	7.51E-07	4.09E-07
Water concentration (mg/L)	4.45E-11	3.57E-07	3.02E-08	5.02E-07	7.90E-07	7.68E-08	4.85E-08	0.00E+00	1.09E-10	4.88E-12
Suspended solids concentration (mg/kg)	3.07E-08	6.11E-04	1.91E-04	3.39E-03	1.02E-02	1.39E-02	1.59E-02	0.00E+00	1.51E-04	6.38E-05
Dissolved organic carbon (mg/kg)	9.80E-08	4.54E-03	7.41E-04	3.10E-02	2.57E-01	5.38E-02	5.56E-02	0.00E+00	1.81E-03	1.45E-03

Sediment Bed	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Fugacity (Pa)	2.35E-14	1.81E-10	4.61E-11	3.80E-10	2.18E-10	6.75E-10	1.31E-10	0.00E+00	1.83E-09	9.95E-10
Pore Water concentration (mg/L)	1.08E-13	8.67E-10	7.34E-11	1.22E-09	1.92E-09	1.87E-10	1.18E-10	0.00E+00	2.65E-13	1.19E-14
Sediment concentration (mg/kg)	4.98E-12	9.90E-08	3.09E-08	5.50E-07	1.65E-06	2.25E-06	2.58E-06	0.00E+00	2.45E-08	1.03E-08

Bioenergetic Inputs	Species	Body Weight	Lipid	Moisture	Caloric Density	GE to ME	Met Energy	Caloric Density	Production	Respiration	Excretion	Caloric Density	Met Energy
		(kg)	(%-dw)	(%)	(kcal/g-dry weight)	Fraction	(kcal/kg-lipid)	(kcal/kg-lipid)	(% of total)	(% of total)	(% of total)	(kcal/g-wt weight)	(kcal/g-wt weight)
Pelagic Community													
Phytoplankton (TL-I)	Algae		10%	84%	2.36	0.6	13748	22913				0.3776	0.22656
Zooplankton (TL-II)	copepods	0.000005	22%	76%	3.6	0.65	10636	16364	18%	24%	58%	0.864	0.5616
Planktivore (TL-III)	herring	0.05	28%	75%	4.9	0.7	12206	17438	20%	60%	20%	1.225	0.8575
Piscivore (TL-IV)	jack	0.5	28%	75%	4.9	0.7	12206	17438	20%	60%	20%	1.225	0.8575
Reef / Vessel Community													
Attached Algae (TL-I)	Algae		10%	84%	2.36	0.6	13748	22913				0.3776	0.22656
Sessile filter feeder (TL-II)	bivalves (w/o shell)	0.05	5%	82%	4.6	0.65	59800	92000	28%	31%	41%	0.828	0.5382
Invertebrate Omnivore (TL-II)	urchin	0.05	29%	82%	4.6	0.65	10310	15862	7%	25%	68%	0.828	0.5382
Invertebrate Forager (TL-III)	crab	1	9%	74%	2.7	0.65	19118	29412	28%	59%	13%	0.702	0.4563
Vertebrate Forager (TL-III)	triggerfish	1	28%	75%	4.9	0.7	12206	17438	20%	60%	20%	1.225	0.8575
Predator (TL-IV)	grouper	1.5	28%	75%	4.9	0.7	12206	17438	20%	60%	20%	0.2	0.14
Benthic Community													
Infaunal invert. (TL-II)	polychaete	0.01	6%	84%	4.6	0.65	50000	76923	71%	26%	3%	0.736	0.4784
Epifaunal invert. (TL-II)	nematode	0.01	6%	82%	4.6	0.65	50000	76923	31%	19%	50%	0.828	0.5382
Forager (TL-III)	lobster	2	9%	74%	2.7	0.65	19118	29412	28%	59%	13%	0.702	0.4563
Predator (TL-IV)	flounder	3	22%	75%	4.9	0.7	15591	22273	20%	60%	20%	1.225	0.8575

PCB MODELING RESULTS - PROSPECTIVE RISK EVALUATION
RISK ESTIMATES FOR Ex-Oriskany CV34 High-End Weight of PCB-Laden Materials
Supplemental Information

Bioenergetic Inputs		Respiration Rate Allometric Regression Parameters			Resp. Rate	Resp. Rate	Consumption	Growth Rate	Consumption	Consumption	
		a	b1	b2	1 / day	gO2 / kg-lipid-day	kcal / kg-lipid-day	1 / day	g-wt weight / g-wt weight-d	kcal / wet weight-da	As a % of body weight
Pelagic Community											
Phytoplankton (TL1)	Algae										
Zooplankton (TL-II)	copepods	0.006375522	0	0.039935335	0.015425453	84.24400867	1286.168071	0.014147849	0.32636028	0.06790967	32.6%
Planktivore (TL-III)	herring	0.0033	-0.227	0.0548	0.004949927	21.1649	129.2512977	0.001482433	0.01616792	0.0090799	1.6%
Piscivore (TL-IV)	jack	0.001118602	-0.55	0.12	0.000630951	2.697821256	16.47524431	0.000188961	0.00139796	0.00115739	0.1%
Reef / Vessel Community											
Attached Algae	Algae										
Sessile filter feeder (TL-II)	bivalves (w/o shell)	0.012	0	0.036	0.024213411	581.8482643	6877.300342	0.020930914	0.24377539	0.0618957	24.4%
Invertebrate Omnivore (TL-II)	urchin	0.000675466	0	0.079181846	0.003163548	13.1069075	192.1012396	0.000847751	0.03471132	0.01002768	3.5%
Invertebrate Forager (TL-III)	crab	0.001158234	0	0.071193202	0.004642088	60.75673491	377.3221989	0.003592107	0.01678102	0.00900593	1.7%
Vertebrate Forager (TL-III)	triggerfish	0.015181024	-0.415	0.061	0.002837229	12.13142452	74.08503521	0.00084971	0.00907693	0.00520447	0.9%
Predator (TL-IV)	grouper	0.00279	-0.355	0.0811	0.001011362	4.324384181	26.40845301	0.000302889	0.00264734	0.00185519	0.3%
Benthic Community											
Infaunal invert. (TL-II)	polychaete	0.001682129	0	0.071034762	0.006721006	135.0382801	1903.064429	0.017565285	0.09800757	0.01820852	9.8%
Epifaunal invert. (TL-II)	nematode	0.001682129	0	0.071034762	0.006721006	135.0382801	2604.19343	0.0104949	0.09262416	0.02803154	9.3%
Forager (TL-III)	lobster	0.0035	-0.13	0.066	0.00471923	61.76639253	383.5925529	0.003651801	0.01899736	0.00915559	1.9%
Predator (TL-IV)	flounder	0.0046	-0.24	0.067	0.002486878	13.58174479	82.94195291	0.000744785	0.00974341	0.00456181	1.0%

Dietary Preferences

	Suspended Solids (Epilimnion)	Suspended Solids (Hypolimnion)	Sediment	Phytoplankton	Zooplankton	Pelagic Plankitivore	Attached Algae	Reef Sessile Filter Feeder	Invertebrate Omnivore	Reef Invertebrate Forager	Reef Vertebrate Forager	Infaunal Benthos	Epifaunal Benthos	Benthic Forager
Pelagic Community														
Phytoplankton (TL1)														
Zooplankton (TL-II)	15%	15%		70%										
Planktivore (TL-III)					100%									
Piscivore (TL-IV)					10%	90%								
Reef / Vessel Community														
Attached Algae														
Sessile filter feeder (TL-II)		10%		80%	10%									
Invertebrate Omnivore (TL-II)							80%	20%						
Invertebrate Forager (TL-III)		5%			5%	5%		35%	50%					
Vertebrate Forager (TL-III)						19%		19%	15%	22%		12.5%	12.5%	
Predator (TL-IV)										15%	60%	8%	8%	8%
Benthic Community														
Infaunal invert. (TL-II)			50%	30%	20%									
Epifaunal invert. (TL-II)			25%	30%	20%							25%		
Forager (TL-III)			5%									50%	45%	
Predator (TL-IV)			2%									20%	20%	58%

Water Exposures		Upper Water Column	Lower Water Column	Vessel Interior	Sediment Pore Water
Pelagic Community					
Phytoplankton (TL1)	Algae	100%			
Zooplankton (TL-II)	copepods	50%	50%		
Planktivore (TL-III)	herring	80%	20%		
Piscivore (TL-IV)	jack	80%	20%		
Reef / Vessel Community					
Attached Algae	Algae		100%		
Sessile filter feeder (TL-II)	bivalves (w/o shell)		100%		
Invertebrate Omnivore (TL-II)	urchin		80%	20%	
Invertebrate Forager (TL-III)	crab		70%	30%	
Vertebrate Forager (TL-III)	triggerfish		70%	30%	
Predator (TL-IV)	grouper		80%	20%	
Benthic Community					
Infaunal invert. (TL-II)	polychaete		20%		80%
Epifaunal invert. (TL-II)	nematode		50%		50%
Forager (TL-III)	lobster		75%		25%
Predator (TL-IV)	flounder		90%		10%

Energy Estimates for Suspended Sediment and Bedded Sediment

	GE	ME	ME	as kcal/g-ww
Sediment (kcal/kg-oc)	11456	6873.6	0.6	0.01099776
Suspended Sediment (kcal/kg-oc)	11456	6873.6	0.6	0.1649664

Respiratory Efficiencies	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Low body weight (<100g)	4.335E-01	8.000E-01	8.000E-01	8.000E-01	4.492E-01	2.582E-01	2.018E-01	1.127E-01	5.303E-02	1.255E-02
High body weight (>100g)	5.000E-01	5.000E-01	5.000E-01	5.000E-01	3.769E-01	2.857E-01	2.526E-01	1.888E-01	1.295E-01	6.299E-02
Dietary Assimilation Efficiencies	27%	46%	53%	62%	69%	69%	68%	59%	44%	16%

Tissue Conc. (mg/kg-lipid)	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Pelagic Community										
Phytoplankton (TL1)	9.143E-13	2.422E-08	1.948E-09	3.159E-08	4.150E-08	1.659E-09	6.797E-10	0.000E+00	3.062E-13	1.097E-15
Zooplankton (TL-II)	7.287E-09	2.706E-04	2.729E-05	5.151E-04	5.109E-04	7.310E-05	6.504E-05	0.000E+00	3.261E-07	4.821E-08
Planktivore (TL-III)	1.647E-09	2.291E-04	4.178E-05	1.528E-03	2.723E-03	4.285E-04	3.717E-04	0.000E+00	1.230E-06	6.474E-08
Piscivore (TL-IV)	4.305E-10	4.039E-05	1.109E-05	8.926E-04	4.773E-03	1.285E-03	1.257E-03	0.000E+00	3.671E-06	8.006E-08
Reef / Vessel Community										
Attached Algae	3.222E-09	8.672E-05	7.339E-06	1.220E-04	1.920E-04	1.868E-05	1.179E-05	0.000E+00	2.653E-08	1.186E-09
Sessile filter feeder (TL-II)	1.037E-07	3.499E-03	3.456E-04	6.498E-03	6.291E-03	5.571E-04	4.034E-04	0.000E+00	1.291E-06	1.401E-07
Invertebrate Omnivore (TL-II)	2.898E-07	2.252E-02	3.328E-03	1.071E-01	1.730E-01	1.224E-02	6.420E-03	0.000E+00	4.488E-06	6.064E-08
Invertebrate Forager (TL-III)	2.192E-06	8.951E-02	1.334E-02	4.503E-01	8.597E-01	6.798E-02	3.772E-02	0.000E+00	4.148E-05	2.711E-06
Vertebrate Forager (TL-III)	2.015E-07	1.416E-02	3.046E-03	1.785E-01	6.347E-01	6.428E-02	3.756E-02	0.000E+00	4.214E-05	1.385E-06
Predator (TL-IV)	1.116E-07	7.257E-03	1.715E-03	1.498E-01	1.156E+00	1.771E-01	1.137E-01	0.000E+00	1.222E-04	2.685E-06
Benthic Community										
Infaunal invert. (TL-II)	2.628E-08	1.032E-03	1.073E-04	2.122E-03	2.130E-03	1.950E-04	1.425E-04	0.000E+00	3.977E-07	2.834E-08
Epifaunal invert. (TL-II)	3.259E-08	1.919E-03	2.289E-04	5.181E-03	5.709E-03	5.472E-04	4.040E-04	0.000E+00	1.015E-06	5.565E-08
Forager (TL-III)	1.903E-08	1.051E-03	1.607E-04	4.856E-03	7.236E-03	6.765E-04	4.610E-04	0.000E+00	7.349E-07	1.686E-08
Predator (TL-IV)	1.685E-09	2.802E-04	7.385E-05	4.574E-03	1.378E-02	1.658E-03	1.171E-03	0.000E+00	1.505E-06	2.213E-08

PCB MODELING RESULTS - PROSPECTIVE RISK EVALUATION

RISK ESTIMATES FOR Ex-Oriskany CV34 High-End Weight of PCB-Laden Materials

Supplemental Information

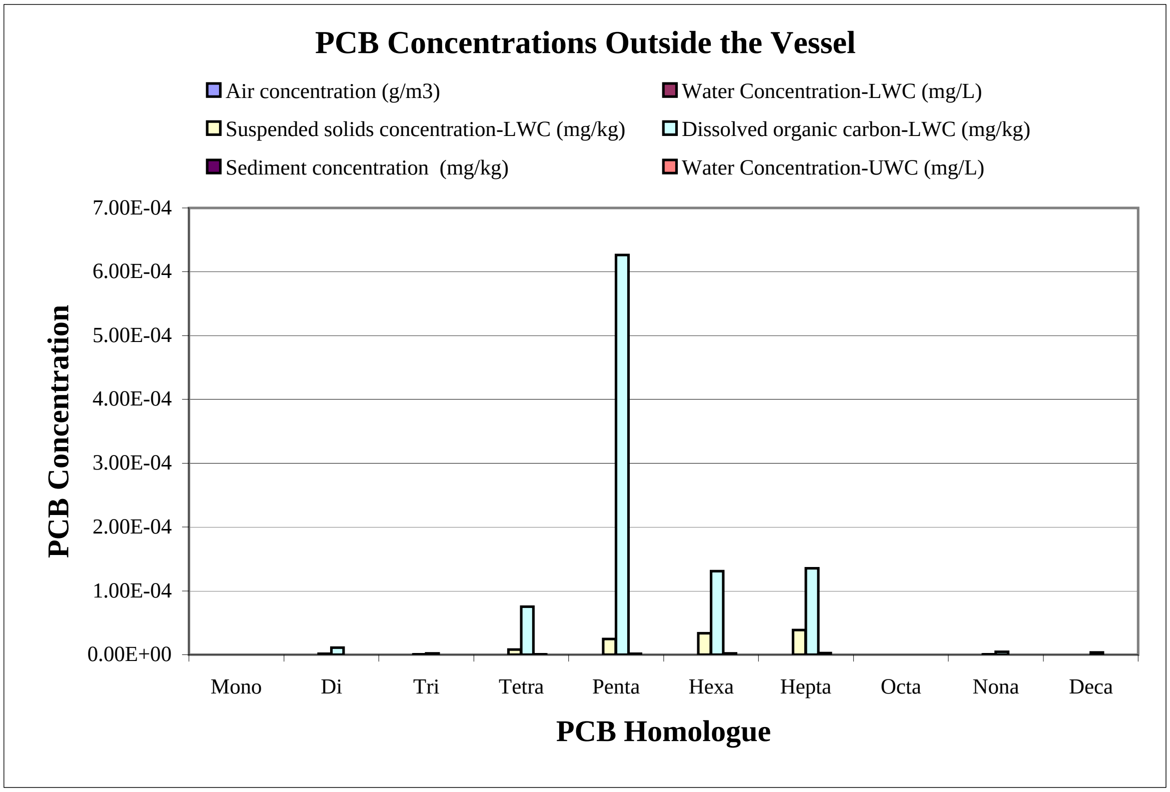
Tissue Conc. (mg/kg-WW)	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca	Total PCB
Pelagic Community											
Phytoplankton (TL1)	1.507E-14	3.991E-10	3.211E-11	5.207E-10	6.838E-10	2.735E-11	1.120E-11	0.000E+00	5.047E-15	1.807E-17	1.674E-09
Zooplankton (TL-II)	3.847E-10	1.429E-05	1.441E-06	2.720E-05	2.698E-05	3.860E-06	3.434E-06	0.000E+00	1.722E-08	2.545E-09	7.722E-05
Planktivore (TL-III)	1.157E-10	1.610E-05	2.935E-06	1.073E-04	1.913E-04	3.010E-05	2.611E-05	0.000E+00	8.639E-08	4.548E-09	3.740E-04
Piscivore (TL-IV)	3.024E-11	2.837E-06	7.791E-07	6.270E-05	3.353E-04	9.028E-05	8.828E-05	0.000E+00	2.579E-07	5.625E-09	5.804E-04
Reef / Vessel Community											
Attached Algae	5.309E-11	1.429E-06	1.209E-07	2.010E-06	3.165E-06	3.078E-07	1.944E-07	0.000E+00	4.372E-10	1.955E-11	7.228E-06
Sessile filter feeder (TL-II)	9.335E-10	3.149E-05	3.110E-06	5.848E-05	5.662E-05	5.014E-06	3.631E-06	0.000E+00	1.162E-08	1.261E-09	1.584E-04
Invertebrate Omnivore (TL-II)	1.513E-08	1.176E-03	1.737E-04	5.591E-03	9.032E-03	6.389E-04	3.351E-04	0.000E+00	2.343E-07	3.166E-09	1.695E-02
Invertebrate Forager (TL-III)	5.231E-08	2.136E-03	3.184E-04	1.075E-02	2.052E-02	1.623E-03	9.003E-04	0.000E+00	9.901E-07	6.469E-08	3.624E-02
Vertebrate Forager (TL-III)	1.415E-08	9.949E-04	2.140E-04	1.254E-02	4.459E-02	4.516E-03	2.638E-03	0.000E+00	2.960E-06	9.732E-08	6.550E-02
Predator (TL-IV)	7.841E-09	5.098E-04	1.205E-04	1.052E-02	8.122E-02	1.244E-02	7.984E-03	0.000E+00	8.585E-06	1.886E-07	1.128E-01
Benthic Community											
Infaunal invert. (TL-II)	2.514E-10	9.875E-06	1.026E-06	2.030E-05	2.038E-05	1.866E-06	1.363E-06	0.000E+00	3.805E-09	2.711E-10	5.482E-05
Epifaunal invert. (TL-II)	3.508E-10	2.066E-05	2.464E-06	5.577E-05	6.146E-05	5.891E-06	4.348E-06	0.000E+00	1.092E-08	5.990E-10	1.506E-04
Forager (TL-III)	4.541E-10	2.508E-05	3.835E-06	1.159E-04	1.727E-04	1.615E-05	1.100E-05	0.000E+00	1.754E-08	4.024E-10	3.447E-04
Predator (TL-IV)	9.265E-11	1.541E-05	4.062E-06	2.516E-04	7.580E-04	9.120E-05	6.440E-05	0.000E+00	8.279E-08	1.217E-09	1.185E-03

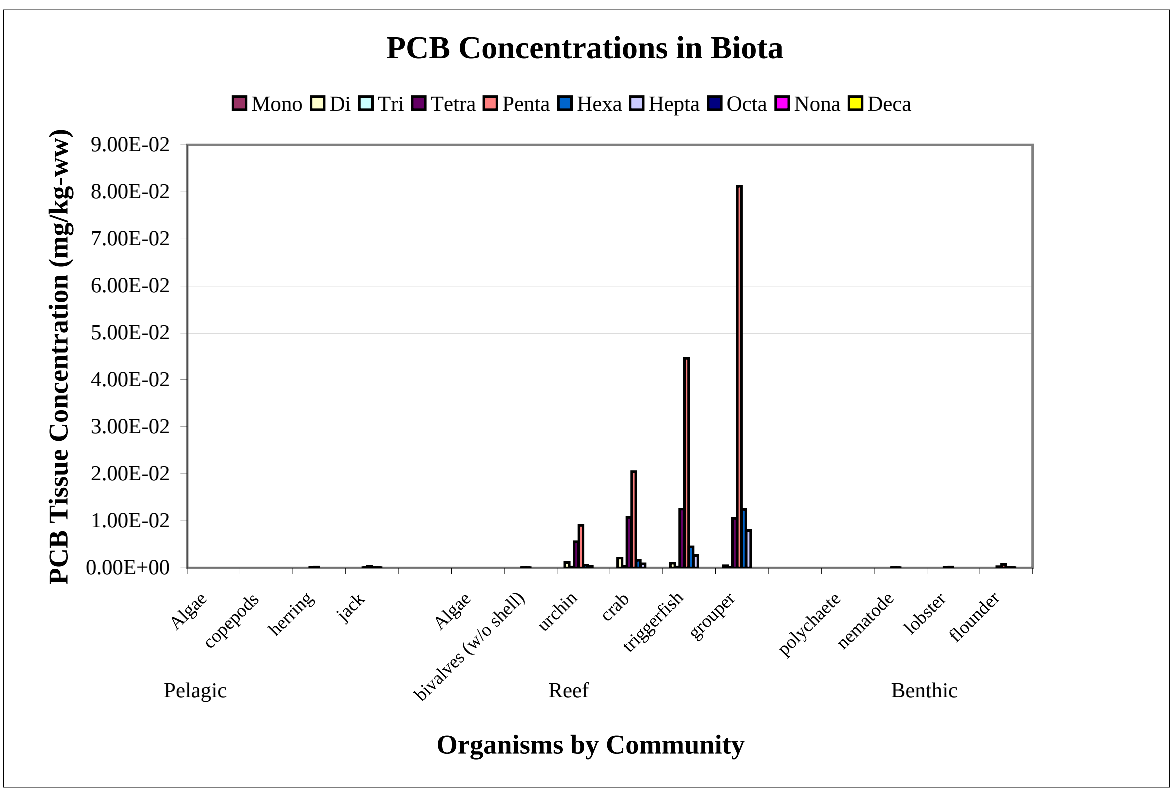
BAFs (L/kg-lipid)	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Pelagic Community										
Phytoplankton (TL1)	2.979E+04	1.000E+05	1.000E+05	1.000E+05	1.000E+05	1.000E+05	1.000E+05	0.000E+00	1.000E+05	1.000E+05
Zooplankton (TL-II)	1.347E+05	6.238E+05	7.436E+05	8.445E+05	5.320E+05	7.826E+05	1.103E+06	0.000E+00	2.458E+06	8.127E+06
Planktivore (TL-III)	7.603E+04	1.320E+06	2.843E+06	6.258E+06	7.083E+06	1.146E+07	1.576E+07	0.000E+00	2.317E+07	2.729E+07
Piscivore (TL-IV)	1.988E+04	2.326E+05	7.548E+05	3.655E+06	1.242E+07	3.439E+07	5.326E+07	0.000E+00	6.917E+07	3.375E+07
Reef / Vessel Community										
Attached Algae	2.979E+04	1.000E+05	1.000E+05	1.000E+05	1.000E+05	1.000E+05	1.000E+05	0.000E+00	1.000E+05	1.000E+05
Sessile filter feeder (TL-II)	9.590E+05	4.034E+06	4.709E+06	5.328E+06	3.276E+06	2.983E+06	3.420E+06	0.000E+00	4.867E+06	1.181E+07
Invertebrate Omnivore (TL-II)	3.226E+04	3.127E+05	5.460E+05	1.057E+06	1.085E+06	7.891E+05	6.556E+05	0.000E+00	2.037E+05	6.157E+04
Invertebrate Forager (TL-III)	1.633E+05	8.319E+05	1.465E+06	2.976E+06	3.608E+06	2.934E+06	2.578E+06	0.000E+00	1.260E+06	1.842E+06
Vertebrate Forager (TL-III)	1.501E+04	1.316E+05	3.345E+05	1.180E+06	2.664E+06	2.774E+06	2.567E+06	0.000E+00	1.280E+06	9.414E+05
Predator (TL-IV)	1.243E+04	1.008E+05	2.815E+05	1.479E+06	7.250E+06	1.142E+07	1.161E+07	0.000E+00	5.547E+06	2.726E+06
Benthic Community										
Infaunal invert. (TL-II)	2.429E+05	1.190E+06	1.462E+06	1.740E+06	1.109E+06	1.044E+06	1.208E+06	0.000E+00	1.499E+06	2.389E+06
Epifaunal invert. (TL-II)	3.013E+05	2.213E+06	3.119E+06	4.248E+06	2.973E+06	2.930E+06	3.425E+06	0.000E+00	3.825E+06	4.691E+06
Forager (TL-III)	1.759E+05	1.212E+06	2.189E+06	3.981E+06	3.768E+06	3.622E+06	3.909E+06	0.000E+00	2.770E+06	1.421E+06
Predator (TL-IV)	1.557E+04	3.231E+05	1.006E+06	3.750E+06	7.177E+06	8.877E+06	9.928E+06	0.000E+00	5.673E+06	1.865E+06

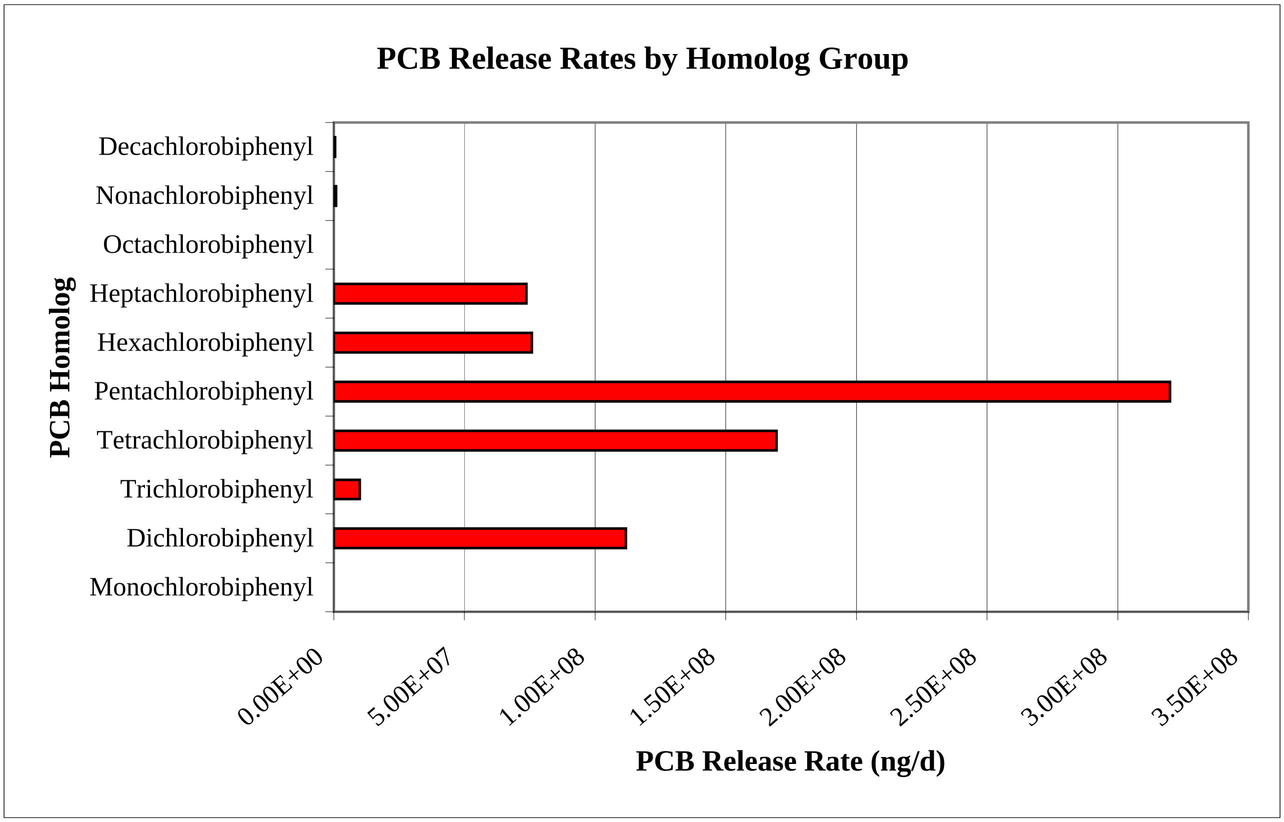
Notes:

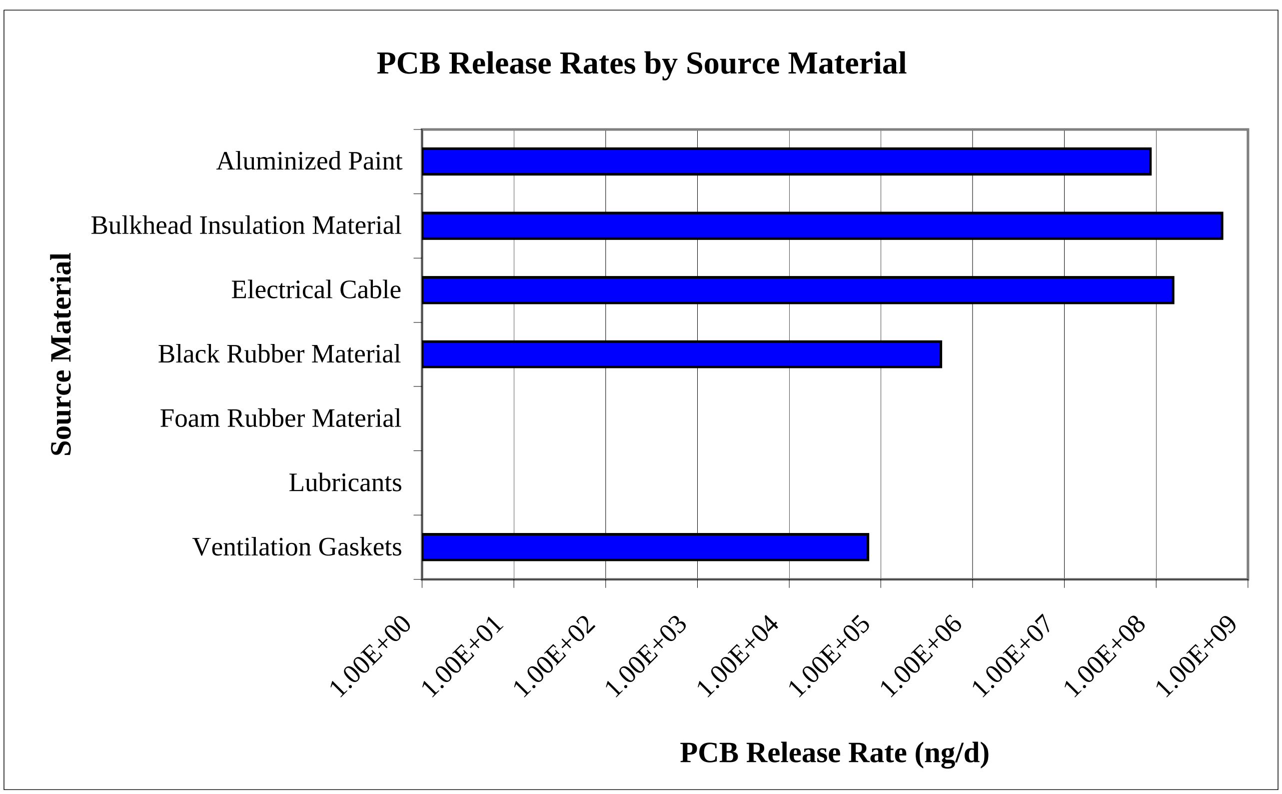
Kow = octanol to water partitioning coefficient, Koc = organic carbon partitioning coefficient, Kdoc = dissolved organic carbon partitioning coefficient

TL = trophic level, ww = wet weight


PCB Concentrations Outside the Vessel
Air concentration (g/m3)
Water Concentration-LWC (mg/L)
Suspended solids concentration-LWC (mg/kg)
Dissolved organic carbon-LWC (mg/kg)
Sediment concentration (mg/kg)
Water Concentration-UWC (mg/L)
PCB Concentration
7.00E-04
6.00E-04
5.00E-04
4.00E-04
3.00E-04
2.00E-04
1.00E-04
0.00E+00
Mono
Di
Tri
Tetra
Penta
Hexa
Hepta
Octa
Nona
Deca
PCB Homologue


PCB Concentrations in Biota
Mono
Di
Tri
Tetra
Penta
Hexa
Hepta
Octa
Nona
Deca
PCB Tissue Concentration (mg/kg-ww)
9.00E-02
8.00E-02
7.00E-02
6.00E-02
5.00E-02
4.00E-02
3.00E-02
2.00E-02
1.00E-02
0.00E+00
Algae
copepods
herring
jack
Algae
bivalves (w/o shell)
urchin
crab
triggerfish
grouper
polychaete
nematode
lobster
flounder
Pelagic
Reef
Benthic
Organisms by Community


PCB Release Rates by Homolog Group
Decachlorobiphenyl
Nonachlorobiphenyl
Octachlorobiphenyl
Heptachlorobiphenyl
Hexachlorobiphenyl
Pentachlorobiphenyl
Tetrachlorobiphenyl
Trichlorobiphenyl
Dichlorobiphenyl
Monochlorobiphenyl
PCB Homolog
0.00E+00
5.00E+07
1.00E+08
1.50E+08
2.00E+08
2.50E+08
3.00E+08
3.50E+08
PCB Release Rate (ng/d)


PCB Release Rates by Source Material
Aluminized Paint
Bulkhead Insulation Material
Electrical Cable
Black Rubber Material
Foam Rubber Material
Lubricants
Ventilation Gaskets
Source Material
1.00E+00
1.00E+01
1.00E+02
1.00E+03
1.00E+04
1.00E+05
1.00E+06
1.00E+07
1.00E+08
1.00E+09
PCB Release Rate (ng/d)

ZOI = 5

PCB MODELING RESULTS - PROSPECTIVE RISK EVALUATION

RISK ESTIMATES FOR Ex-Oriskany CV34

	Cancer Risk Adult & Child		Hazard Adult & Child		Cancer Risk Child		Hazard Child	
RISK ESTIMATES	RME	CTE	RME	CTE	RME	CTE	RME	CTE
Benthic fish (flounder)	4.23E-08	3.28E-09	2.47E-03	5.66E-04	1.24E-08	2.52E-09	3.62E-03	6.53E-04
Benthic shellfish (lobster)	1.23E-08	9.53E-10	7.18E-04	1.65E-04	3.61E-09	7.33E-10	1.05E-03	1.90E-04
Pelagic fish (jack)	2.07E-08	1.61E-09	1.21E-03	2.78E-04	6.08E-09	1.23E-09	1.77E-03	3.20E-04
Reef fish TL-IV (grouper)	6.86E-06	5.31E-07	4.00E-01	9.18E-02	2.01E-06	4.08E-07	5.87E-01	1.06E-01
Reef fish TL-III (triggerfish)	3.98E-06	3.08E-07	2.32E-01	5.33E-02	1.17E-06	2.37E-07	3.41E-01	6.14E-02
Reef shellfish (crab)	2.21E-06	1.71E-07	1.29E-01	2.95E-02	6.48E-07	1.31E-07	1.89E-01	3.41E-02

PREDICTED EXPOSURE CONCENTRATIONS (mg/kg in fresh weight)	
Benthic fish (flounder)	6.88E-04
Benthic shellfish (lobster)	2.00E-04
Pelagic fish (jack)	3.37E-04
Reef fish TL-IV (grouper)	1.11E-01
Reef fish TL-III (triggerfish)	6.47E-02
Reef shellfish (crab)	3.59E-02

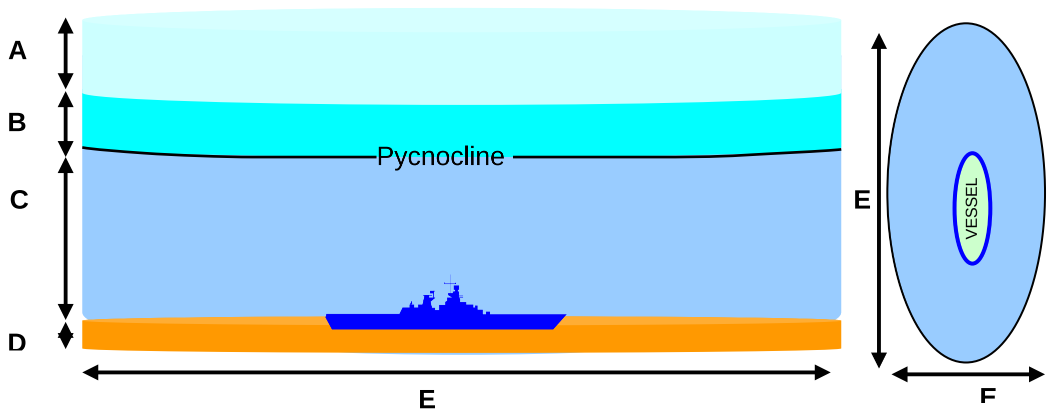
RISK INPUTS - Adult	RME	CTE
Body Weight (BWa) (kg)	70	70
Exposure Frequency (EFa) (days)	365	365
Exposure Duration (EDa) (years)	24	3
Ingestion Rate (IRa) (kg/day)	0.0261	0.0072
Averaging Time for cancer (ATc)	25550	25550
Averaging Time for noncancer (ATnc-adult)	8760	1095
Slope Factor (mg/kg-day)	2	1
Reference dose for PCBs (RfD) (mg/kg-day)	2.00E-05	4.50E-05
Fractional Ingestion factor (FI)	0.17	0.25
Ingestion Rates Based on Data from	Gulf Coast	

RISK INPUTS - Child	RME	CTE
Body Weight (BWc) (kg)	15	15
Exposure Frequency (EFc) (days)	365	365
Exposure Duration (EDc) (years)	6	6
Ingestion Rate (IRc) (kg/day)	0.0092916	0.0025632
Averaging Time for cancer (ATc)	25550	25550
Averaging Time for noncancer (ATnc-child)	2190	2190
Slope Factor (mg/kg-day)	2	1
Reference dose for PCBs (RfD) (mg/kg-day)	2.00E-05	4.50E-05
Fractional Ingestion factor (FI)	0.17	0.25
Child - Adult IR scaling factor	0.356	

Zone of Influence Multiplier	5
Scenario run on	5/11/05 13:38

PCB-LADEN MATERIAL INPUTS	Fraction PCB	Release Rate (ng/g-d)	kg Material Onboard	PCB Release (ng/day)
Ventilation Gaskets	3.14E-05	1.58E+03	1.46E+03	7.23E+04
Lubricants	1.03E-04	2.20E+03	0.00E+00	0.00E+00
Foam Rubber Material	7.60E-03	2.62E+00	0.00E+00	0.00E+00
Black Rubber Material	5.29E-05	1.58E+03	5.40E+03	4.50E+05
Electrical Cable	1.85E-03	2.79E+02	2.96E+05	1.53E+08
Bulkhead Insulation Material	5.37E-04	6.76E+04	1.44E+04	5.22E+08
Aluminum Paint	2.00E-05	1.11E+04	3.87E+05	8.62E+07
Total				7.62E+08

Ex-Oriskany CV34	
Displacement (tons)	27100
Length (ft)	888
Beam (ft)	120



ZOI =	5	
Spatial Footprint on Ocean Floor		
	3.89E+04	m2
	1.50E-02	mile2
Modeled Dimensions Outside the Vessel		
A	1.00E+01	m
B	1.50E+01	m
C	5.00E+01	m
D	1.00E-01	m
E	3.68E+02	m
F	1.34E+02	m
Volumes		
Air Column		
Air	3.89E+05	m3
Upper Water Column		
Water	5.83E+05	m3
TSS	3.89E+00	m3
Lower Water Column		
Water	1.89E+06	m3
TSS	1.26E+01	m3
Inside Vessel		
Water	5.38E+04	m3
TSS	3.59E-01	m3
Sediment Bed		
Sediment	3.11E+03	m3

Abiotic Inputs

Air Column

Active air space height above water column (m)	10

Total PCB concentrations

Air Column

Air	9.68E-17	g/m3

Air current (m/h)	13677
Upper Water Column	
Temperature (°C)	24.5
Water depth (m)	15
Total suspended solids (mg/L)	10
Dissolved organic carbon (mg/L)	0.6
Dissolved oxygen (mg/L)	6.12
Lower Water Column	
Temperature (°C)	19.5
Water depth (m)	50
Total suspended solids (mg/L)	10
Dissolved organic carbon (mg/L)	0.6
Dissolved oxygen (mg/L)	4.59
Inside Vessel	
Temperature (°C)	19.5
Total suspended solids (mg/L)	10
Dissolved organic carbon (mg/L)	0.6
Dissolved oxygen (mg/L)	4.59
Sediment Bed	
Sediment density (g/cm3)	1.5
Active sediment depth (m)	0.1
Sediment fraction organic carbon	0.01
All Regions	
Suspended solids density (g/cm3)	1.5
Suspended solids fraction organic carbon	0.15
Dissolved organic carbon density (g/cm3)	1
Water current - to out of the ZOI (m/h)	926
Water current - inside to outside the vessel (m/h)	9.26

Upper Water Column		
Freely dissolved in water	9.32E-13	mg/L
Suspended solids	1.22E-08	mg/kg
Dissolved organic carbon	1.63E-07	mg/kg
Lower Water Column		
Freely dissolved in water	2.55E-09	mg/L
Suspended solids	6.27E-05	mg/kg
Dissolved organic carbon	5.74E-04	mg/kg
Inside Vessel		
Freely dissolved in water	1.80E-06	mg/L
Suspended solids	4.44E-02	mg/kg
Dissolved organic carbon	4.06E-01	mg/kg
Sediment Bed		
Freely dissolved in pore water	2.55E-09	mg/L
Bedded sediment	4.18E-06	mg/kg
Dissolved organic carbon in pore water	5.74E-04	mg/kg

Total PCB concentrations in biota			**Percent Exposures**	
Pelagic Community			Upper WC	Lower WC
Phytoplankton (TL-I)	1.54E-09	mg/kg	100%	0%
Zooplankton (TL-II)	4.48E-05	mg/kg	50%	50%
Planktivore (TL-III)	2.17E-04	mg/kg	80%	20%
Piscivore (TL-IV)	3.37E-04	mg/kg	80%	20%
Reef / Vessel Community			Lower WC	Vessel Int.
Attached Algae (TL-I)	4.20E-06	mg/kg	100%	0%
Sessile filter feeder (TL-II)	9.19E-05	mg/kg	100%	0%
Invertebrate Omnivore (TL-II)	1.67E-02	mg/kg	80%	20%
Invertebrate Forager (TL-III)	3.59E-02	mg/kg	70%	30%
Vertebrate Forager (TL-III)	6.47E-02	mg/kg	70%	30%
Predator (TL-IV)	1.11E-01	mg/kg	80%	20%
Benthic Community			Lower WC	Pore Water
Infaunal invert. (TL-II)	3.18E-05	mg/kg	20%	80%
Epifaunal invert. (TL-II)	8.74E-05	mg/kg	50%	50%
Forager (TL-III)	2.00E-04	mg/kg	75%	25%
Predator (TL-IV)	6.88E-04	mg/kg	90%	10%

PCB MODELING RESULTS - PROSPECTIVE RISK EVALUATION
RISK ESTIMATES FOR Ex-Oriskany CV34 High-End Weight of PCB-Laden Materials
Supplemental Information

Scenario Run on 10/21/2004 14:10

PCB Homolog	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Molecular Weight (g/mol)	1.89E+02	2.23E+02	2.58E+02	2.92E+02	3.26E+02	3.61E+02	3.95E+02	4.30E+02	4.64E+02	4.99E+02
Solubility (mg/L)	2.91E+00	6.78E-01	8.14E-02	6.67E-02	2.61E-02	9.50E-04	2.30E-04	2.11E-08	4.02E-09	1.69E-10
Solubility (mol/m^3)	1.54E-02	3.04E-03	3.16E-04	2.28E-04	8.00E-05	2.63E-06	5.82E-07	4.91E-11	8.65E-12	3.38E-13
Vapor Pressure (Pa)	6.32E-01	1.41E-01	5.11E-02	2.08E-02	2.96E-03	3.43E-03	2.56E-04	8.65E-05	2.77E-05	1.41E-05
Henry's (Pa-m^3/mol)	4.10E+01	4.65E+01	1.62E+02	9.10E+01	3.70E+01	1.30E+03	4.40E+02	1.76E+06	3.20E+06	4.18E+07
$log_{10}K_{ow}$ =	4.47	5.24	5.52	5.92	6.50	6.98	7.19	7.70	8.35	9.60
$log_{10}K_{oc}$ =	3.66	4.06	4.63	4.65	4.94	6.08	6.34	6.46	6.97	7.94
$log_{10}K_{doc}$ =	3.34	4.11	4.39	4.79	5.51	5.85	6.06	6.57	7.22	8.47
Chemical emission rate (g/day)	1.37E-05	1.12E-01	9.95E-03	1.69E-01	3.20E-01	7.57E-02	7.37E-02	0.00E+00	8.28E-04	4.62E-04
Chemical emission rate (mol/hr)	3.03E-09	2.09E-05	1.61E-06	2.42E-05	4.08E-05	8.74E-06	7.77E-06	0.00E+00	7.43E-08	3.86E-08
Biodegradation in sediment (1/hr)	0	0	0	0	0	0	0	0	0	0
Biodegradation in water (1/hr)	0	0	0	0	0	0	0	0	0	0

	Ventilation Gaskets	Lubricants	Foam Rubber Material	Black Rubber Material	Electrical Cable	Bulkhead Insulation Material	Aluminized Paint
Fraction PCB in Material (wt/wt)	0.0000314	0.000103	0.76%	0.0000529	0.00185	0.000537	0.00002
Material Mass Onboard (kg)	1459	0	0	5397	296419	14379	386528
Total PCBs (kg)	0.0458126	0	0	0.2855013	548.37515	7.721523	7.73056
Total PCB Release rate (ng/g-PCB per day)	1.58E+03	2.20E+03	2.62E+00	1.58E+03	2.79E+02	6.76E+04	1.11E+04

Release Rates in nanograms PCB per gram of PCB within the Material	Ventilation Gaskets	Lubricants	Foam Rubber Material	Black Rubber Material	Electrical Cable	Bulkhead Insulation Material	Aluminized Paint
Monochlorobiphenyl	4.14E+01	3.47E+01	0.00E+00	4.14E+01	0.00E+00	0.00E+00	0.00E+00
Dichlorobiphenyl	1.27E+03	1.72E+02	3.08E-02	1.27E+03	2.03E+02	5.36E+00	0.00E+00
Trichlorobiphenyl	5.66E+01	8.97E+01	7.63E-02	5.66E+01	1.14E+00	9.44E+02	2.61E+02
Tetrachlorobiphenyl	1.44E+02	1.08E+03	1.29E+00	1.44E+02	1.57E+01	2.07E+04	1.23E+02
Pentachlorobiphenyl	6.31E+01	6.60E+02	3.90E-02	6.31E+01	1.80E+01	3.79E+04	2.24E+03
Hexachlorobiphenyl	0.00E+00	9.42E+01	5.34E-01	0.00E+00	2.41E+01	6.76E+03	1.33E+03
Heptachlorobiphenyl	5.04E+00	7.17E+01	6.46E-01	5.04E+00	1.47E+01	1.30E+03	7.19E+03
Octachlorobiphenyl	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Nonachlorobiphenyl	0.00E+00	0.00E+00	1.72E-03	0.00E+00	1.51E+00	0.00E+00	0.00E+00
Decachlorobiphenyl	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.43E-01	0.00E+00	0.00E+00
Total	**1.58E+03**	**2.20E+03**	**2.62E+00**	**1.58E+03**	**2.79E+02**	**6.76E+04**	**1.11E+04**

Release Rates in nanograms PCB per Day	Ventilation Gaskets	Lubricants	Foam Rubber Material	Black Rubber Material	Electrical Cable	Bulkhead Insulation Material	Aluminized Paint	Total
Monochlorobiphenyl	1.90E+03	0.00E+00	0.00E+00	1.18E+04	0.00E+00	0.00E+00	0.00E+00	1.37E+04
Dichlorobiphenyl	5.80E+04	0.00E+00	0.00E+00	3.62E+05	1.11E+08	4.14E+04	0.00E+00	1.12E+08
Trichlorobiphenyl	2.59E+03	0.00E+00	0.00E+00	1.62E+04	6.25E+05	7.29E+06	2.02E+06	9.95E+06
Tetrachlorobiphenyl	6.60E+03	0.00E+00	0.00E+00	4.11E+04	8.61E+06	1.60E+08	9.51E+05	1.69E+08
Pentachlorobiphenyl	2.89E+03	0.00E+00	0.00E+00	1.80E+04	9.87E+06	2.93E+08	1.73E+07	3.20E+08
Hexachlorobiphenyl	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.32E+07	5.22E+07	1.03E+07	7.57E+07
Heptachlorobiphenyl	2.31E+02	0.00E+00	0.00E+00	1.44E+03	8.06E+06	1.01E+07	5.56E+07	7.37E+07
Octachlorobiphenyl	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Nonachlorobiphenyl	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.28E+05	0.00E+00	0.00E+00	8.28E+05
Decachlorobiphenyl	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.62E+05	0.00E+00	0.00E+00	4.62E+05
Total	7.23E+04	0.00E+00	0.00E+00	4.50E+05	1.53E+08	5.22E+08	8.62E+07	7.62E+08

Air	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Fugacity (Pa)	4.65E-20	2.86E-16	1.89E-17	2.52E-16	2.76E-16	9.75E-18	3.48E-18	0.00E+00	1.23E-21	3.97E-24
Air concentration (g/m3)	3.58E-21	2.60E-17	1.98E-18	3.00E-17	3.67E-17	1.43E-18	5.60E-19	0.00E+00	2.33E-22	8.06E-25

Upper Water Column	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Fugacity (Pa)	6.12E-18	4.63E-14	1.12E-14	9.04E-14	4.32E-14	5.50E-14	6.95E-15	0.00E+00	1.94E-14	8.44E-16
Water concentration (mg/L)	2.82E-17	2.22E-13	1.79E-14	2.90E-13	3.81E-13	1.52E-14	6.24E-15	0.00E+00	2.81E-18	1.01E-20
Suspended solids concentration (mg/kg)	1.95E-14	3.80E-10	1.13E-10	1.96E-09	4.92E-09	2.75E-09	2.05E-09	0.00E+00	3.89E-12	1.32E-13
Dissolved organic carbon (mg/kg)	6.21E-14	2.83E-09	4.39E-10	1.79E-08	1.24E-07	1.07E-08	7.15E-09	0.00E+00	4.67E-11	2.99E-12

Lower Water Column	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Fugacity (Pa)	1.37E-14	1.05E-10	2.67E-11	2.21E-10	1.27E-10	3.92E-10	7.63E-11	0.00E+00	1.06E-09	5.78E-10
Water concentration (mg/L)	6.28E-14	5.03E-10	4.26E-11	7.08E-10	1.11E-09	1.08E-10	6.85E-11	0.00E+00	1.54E-13	6.89E-15
Suspended solids concentration (mg/kg)	4.34E-11	8.62E-07	2.69E-07	4.79E-06	1.44E-05	1.96E-05	2.25E-05	0.00E+00	2.13E-07	9.01E-08
Dissolved organic carbon (mg/kg)	1.38E-10	6.41E-06	1.05E-06	4.38E-05	3.63E-04	7.60E-05	7.85E-05	0.00E+00	2.56E-06	2.04E-06

Inside the Vessel	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Fugacity (Pa)	9.67E-12	7.43E-08	1.89E-08	1.56E-07	8.96E-08	2.77E-07	5.40E-08	0.00E+00	7.51E-07	4.09E-07
Water concentration (mg/L)	4.45E-11	3.57E-07	3.02E-08	5.02E-07	7.90E-07	7.68E-08	4.85E-08	0.00E+00	1.09E-10	4.88E-12
Suspended solids concentration (mg/kg)	3.07E-08	6.11E-04	1.91E-04	3.39E-03	1.02E-02	1.39E-02	1.59E-02	0.00E+00	1.51E-04	6.38E-05
Dissolved organic carbon (mg/kg)	9.80E-08	4.54E-03	7.41E-04	3.10E-02	2.57E-01	5.38E-02	5.56E-02	0.00E+00	1.81E-03	1.45E-03

Sediment Bed	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Fugacity (Pa)	1.37E-14	1.05E-10	2.67E-11	2.21E-10	1.27E-10	3.92E-10	7.63E-11	0.00E+00	1.06E-09	5.78E-10
Pore Water concentration (mg/L)	6.28E-14	5.03E-10	4.26E-11	7.08E-10	1.11E-09	1.08E-10	6.85E-11	0.00E+00	1.54E-13	6.89E-15
Sediment concentration (mg/kg)	2.89E-12	5.75E-08	1.80E-08	3.19E-07	9.60E-07	1.30E-06	1.50E-06	0.00E+00	1.42E-08	6.01E-09

Bioenergetic Inputs

	Species	Body Weight	Lipid	Moisture	Caloric Density	GE to ME	Met Energy	Caloric Density	Production	Respiration	Excretion	Caloric Density	Met Energy
		(kg)	(%-dw)	(%)	(kcal/g-dry weight)	Fraction	(kcal/kg-lipid)	(kcal/kg-lipid)	(% of total)	(% of total)	(% of total)	(kcal/g-wt weight)	(kcal/g-wt weight)
Pelagic Community													
Phytoplankton (TL-I)	Algae		10%	84%	2.36	0.6	13748	22913				0.3776	0.22656
Zooplankton (TL-II)	copepods	0.000005	22%	76%	3.6	0.65	10636	16364	18%	24%	58%	0.864	0.5616
Planktivore (TL-III)	herring	0.05	28%	75%	4.9	0.7	12206	17438	20%	60%	20%	1.225	0.8575
Piscivore (TL-IV)	jack	0.5	28%	75%	4.9	0.7	12206	17438	20%	60%	20%	1.225	0.8575
Reef / Vessel Community													
Attached Algae (TL-I)	Algae		10%	84%	2.36	0.6	13748	22913				0.3776	0.22656
Sessile filter feeder (TL-II)	bivalves (w/o shell)	0.05	5%	82%	4.6	0.65	59800	92000	28%	31%	41%	0.828	0.5382
Invertebrate Omnivore (TL-II)	urchin	0.05	29%	82%	4.6	0.65	10310	15862	7%	25%	68%	0.828	0.5382
Invertebrate Forager (TL-III)	crab	1	9%	74%	2.7	0.65	19118	29412	28%	59%	13%	0.702	0.4563
Vertebrate Forager (TL-III)	triggerfish	1	28%	75%	4.9	0.7	12206	17438	20%	60%	20%	1.225	0.8575
Predator (TL-IV)	grouper	1.5	28%	75%	4.9	0.7	12206	17438	20%	60%	20%	0.2	0.14
Benthic Community													
Infaunal invert. (TL-II)	polychaete	0.01	6%	84%	4.6	0.65	50000	76923	71%	26%	3%	0.736	0.4784
Epifaunal invert. (TL-II)	nematode	0.01	6%	82%	4.6	0.65	50000	76923	31%	19%	50%	0.828	0.5382
Forager (TL-III)	lobster	2	9%	74%	2.7	0.65	19118	29412	28%	59%	13%	0.702	0.4563
Predator (TL-IV)	flounder	3	22%	75%	4.9	0.7	15591	22273	20%	60%	20%	1.225	0.8575

PCB MODELING RESULTS - PROSPECTIVE RISK EVALUATION
RISK ESTIMATES FOR Ex-Oriskany CV34 High-End Weight of PCB-Laden Materials
Supplemental Information

Bioenergetic Inputs		Respiration Rate Allometric Regression Parameters			Resp. Rate	Resp. Rate	Consumption	Growth Rate	Consumption	Consumption	
		a	b1	b2	1 / day	gO2 / kg-lipid-day	kcal / kg-lipid-day	1 / day	g-wt weight / g-wt weight-d	kcal / wet weight-da	As a % of body weight
Pelagic Community											
Phytoplankton (TL1)	Algae										
Zooplankton (TL-II)	copepods	0.006375522	0	0.039935335	0.015425453	84.24400867	1286.168071	0.014147849	0.32636028	0.06790967	32.6%
Planktivore (TL-III)	herring	0.0033	-0.227	0.0548	0.004949927	21.1649	129.2512977	0.001482433	0.01616792	0.0090799	1.6%
Piscivore (TL-IV)	jack	0.001118602	-0.55	0.12	0.000630951	2.697821256	16.47524431	0.000188961	0.00139796	0.00115739	0.1%
Reef / Vessel Community											
Attached Algae	Algae										
Sessile filter feeder (TL-II)	bivalves (w/o shell)	0.012	0	0.036	0.024213411	581.8482643	6877.300342	0.020930914	0.24377539	0.0618957	24.4%
Invertebrate Omnivore (TL-II)	urchin	0.000675466	0	0.079181846	0.003163548	13.1069075	192.1012396	0.000847751	0.03471132	0.01002768	3.5%
Invertebrate Forager (TL-III)	crab	0.001158234	0	0.071193202	0.004642088	60.75673491	377.3221989	0.003592107	0.01678102	0.00900593	1.7%
Vertebrate Forager (TL-III)	triggerfish	0.015181024	-0.415	0.061	0.002837229	12.13142452	74.08503521	0.00084971	0.00907693	0.00520447	0.9%
Predator (TL-IV)	grouper	0.00279	-0.355	0.0811	0.001011362	4.324384181	26.40845301	0.000302889	0.00264734	0.00185519	0.3%
Benthic Community											
Infaunal invert. (TL-II)	polychaete	0.001682129	0	0.071034762	0.006721006	135.0382801	1903.064429	0.017565285	0.09800757	0.01820852	9.8%
Epifaunal invert. (TL-II)	nematode	0.001682129	0	0.071034762	0.006721006	135.0382801	2604.19343	0.0104949	0.09262416	0.02803154	9.3%
Forager (TL-III)	lobster	0.0035	-0.13	0.066	0.00471923	61.76639253	383.5925529	0.003651801	0.01899736	0.00915559	1.9%
Predator (TL-IV)	flounder	0.0046	-0.24	0.067	0.002486878	13.58174479	82.94195291	0.000744785	0.00974341	0.00456181	1.0%

Dietary Preferences	Suspended Solids (Epilimnion)	Suspended Solids (Hypolimnion)	Sediment	Phytoplankton	Zooplankton	Pelagic Plankitivore	Attached Algae	Reef Sessile Filter Feeder	Invertebrate Omnivore	Reef Invertebrate Forager	Reef Vertebrate Forager	Infaunal Benthos	Epifaunal Benthos	Benthic Forager
Pelagic Community														
Phytoplankton (TL1)														
Zooplankton (TL-II)	15%	15%		70%										
Planktivore (TL-III)					100%									
Piscivore (TL-IV)					10%	90%								
Reef / Vessel Community														
Attached Algae														
Sessile filter feeder (TL-II)		10%		80%	10%									
Invertebrate Omnivore (TL-II)							80%	20%						
Invertebrate Forager (TL-III)		5%			5%	5%		35%	50%					
Vertebrate Forager (TL-III)						19%		19%	15%	22%		12.5%	12.5%	
Predator (TL-IV)										15%	60%	8%	8%	8%
Benthic Community														
Infaunal invert. (TL-II)			50%	30%	20%									
Epifaunal invert. (TL-II)			25%	30%	20%							25%		
Forager (TL-III)			5%									50%	45%	
Predator (TL-IV)			2%									20%	20%	58%

Water Exposures		Upper Water Column	Lower Water Column	Vessel Interior	Sediment Pore Water
Pelagic Community					
Phytoplankton (TL1)	Algae	100%			
Zooplankton (TL-II)	copepods	50%	50%		
Planktivore (TL-III)	herring	80%	20%		
Piscivore (TL-IV)	jack	80%	20%		
Reef / Vessel Community					
Attached Algae	Algae		100%		
Sessile filter feeder (TL-II)	bivalves (w/o shell)		100%		
Invertebrate Omnivore (TL-II)	urchin		80%	20%	
Invertebrate Forager (TL-III)	crab		70%	30%	
Vertebrate Forager (TL-III)	triggerfish		70%	30%	
Predator (TL-IV)	grouper		80%	20%	
Benthic Community					
Infaunal invert. (TL-II)	polychaete		20%		80%
Epifaunal invert. (TL-II)	nematode		50%		50%
Forager (TL-III)	lobster		75%		25%
Predator (TL-IV)	flounder		90%		10%

Energy Estimates for Suspended Sediment and Bedded Sediment	GE	ME	ME	as kcal/g-ww
Sediment (kcal/kg-oc)	11456	6873.6	0.6	0.01099776
Suspended Sediment (kcal/kg-oc)	11456	6873.6	0.6	0.1649664

Respiratory Efficiencies	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Low body weight (<100g)	4.335E-01	8.000E-01	8.000E-01	8.000E-01	4.492E-01	2.582E-01	2.018E-01	1.127E-01	5.303E-02	1.255E-02
High body weight (>100g)	5.000E-01	5.000E-01	5.000E-01	5.000E-01	3.769E-01	2.857E-01	2.526E-01	1.888E-01	1.295E-01	6.299E-02
Dietary Assimilation Efficiencies	27%	46%	53%	62%	69%	69%	68%	59%	44%	16%

Tissue Conc. (mg/kg-lipid)	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Pelagic Community										
Phytoplankton (TL1)	8.387E-13	2.222E-08	1.787E-09	2.899E-08	3.807E-08	1.523E-09	6.239E-10	0.000E+00	2.811E-13	1.007E-15
Zooplankton (TL-II)	4.231E-09	1.571E-04	1.585E-05	2.991E-04	2.967E-04	4.244E-05	3.776E-05	0.000E+00	1.893E-07	2.799E-08
Planktivore (TL-III)	9.564E-10	1.331E-04	2.426E-05	8.873E-04	1.581E-03	2.488E-04	2.158E-04	0.000E+00	7.140E-07	3.758E-08
Piscivore (TL-IV)	2.501E-10	2.346E-05	6.441E-06	5.183E-04	2.772E-03	7.462E-04	7.296E-04	0.000E+00	2.131E-06	4.648E-08
Reef / Vessel Community										
Attached Algae	1.870E-09	5.035E-05	4.260E-06	7.080E-05	1.115E-04	1.084E-05	6.847E-06	0.000E+00	1.540E-08	6.887E-10
Sessile filter feeder (TL-II)	6.022E-08	2.031E-03	2.006E-04	3.773E-03	3.652E-03	3.235E-04	2.342E-04	0.000E+00	7.497E-07	8.135E-08
Invertebrate Omnivore (TL-II)	2.883E-07	2.235E-02	3.298E-03	1.060E-01	1.708E-01	1.202E-02	6.275E-03	0.000E+00	4.231E-06	5.249E-08
Invertebrate Forager (TL-III)	2.186E-06	8.904E-02	1.325E-02	4.464E-01	8.506E-01	6.702E-02	3.707E-02	0.000E+00	4.056E-05	2.689E-06
Vertebrate Forager (TL-III)	2.009E-07	1.406E-02	3.019E-03	1.767E-01	6.272E-01	6.326E-02	3.683E-02	0.000E+00	4.112E-05	1.369E-06
Predator (TL-IV)	1.112E-07	7.216E-03	1.703E-03	1.483E-01	1.143E+00	1.745E-01	1.116E-01	0.000E+00	1.199E-04	2.665E-06
Benthic Community										
Infaunal invert. (TL-II)	1.525E-08	5.992E-04	6.227E-05	1.232E-03	1.237E-03	1.132E-04	8.273E-05	0.000E+00	2.309E-07	1.645E-08
Epifaunal invert. (TL-II)	1.892E-08	1.114E-03	1.329E-04	3.008E-03	3.315E-03	3.177E-04	2.345E-04	0.000E+00	5.892E-07	3.231E-08
Forager (TL-III)	1.105E-08	6.101E-04	9.328E-05	2.819E-03	4.201E-03	3.928E-04	2.676E-04	0.000E+00	4.266E-07	9.788E-09
Predator (TL-IV)	9.779E-10	1.627E-04	4.287E-05	2.656E-03	8.002E-03	9.627E-04	6.798E-04	0.000E+00	8.739E-07	1.285E-08

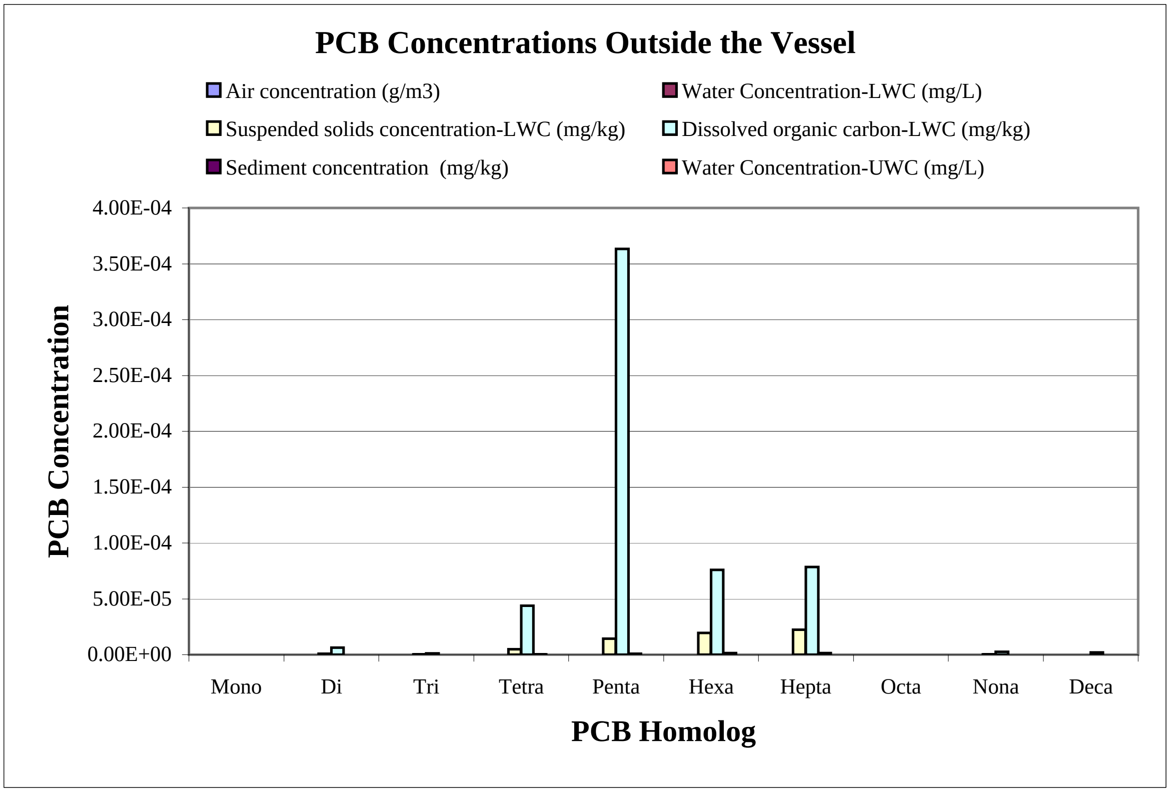
Tissue Conc. (mg/kg-WW)	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca	Total PCB
Pelagic Community											
Phytoplankton (TL1)	1.382E-14	3.661E-10	2.946E-11	4.777E-10	6.275E-10	2.510E-11	1.028E-11	0.000E+00	4.633E-15	1.659E-17	1.536E-09
Zooplankton (TL-II)	2.234E-10	8.295E-06	8.368E-07	1.579E-05	1.567E-05	2.241E-06	1.994E-06	0.000E+00	9.996E-09	1.478E-09	4.484E-05
Planktivore (TL-III)	6.719E-11	9.348E-06	1.704E-06	6.233E-05	1.111E-04	1.748E-05	1.516E-05	0.000E+00	5.016E-08	2.640E-09	2.172E-04
Piscivore (TL-IV)	1.757E-11	1.648E-06	4.525E-07	3.641E-05	1.947E-04	5.242E-05	5.125E-05	0.000E+00	1.497E-07	3.265E-09	3.371E-04
Reef / Vessel Community											
Attached Algae	3.082E-11	8.297E-07	7.021E-08	1.167E-06	1.837E-06	1.787E-07	1.128E-07	0.000E+00	2.538E-10	1.135E-11	4.196E-06
Sessile filter feeder (TL-II)	5.420E-10	1.828E-05	1.806E-06	3.395E-05	3.287E-05	2.911E-06	2.108E-06	0.000E+00	6.748E-09	7.322E-10	9.194E-05
Invertebrate Omnivore (TL-II)	1.505E-08	1.167E-03	1.722E-04	5.534E-03	8.918E-03	6.275E-04	3.276E-04	0.000E+00	2.209E-07	2.740E-09	1.675E-02
Invertebrate Forager (TL-III)	5.217E-08	2.125E-03	3.163E-04	1.065E-02	2.030E-02	1.600E-03	8.848E-04	0.000E+00	9.682E-07	6.418E-08	3.588E-02
Vertebrate Forager (TL-III)	1.411E-08	9.880E-04	2.121E-04	1.241E-02	4.406E-02	4.444E-03	2.587E-03	0.000E+00	2.889E-06	9.615E-08	6.471E-02
Predator (TL-IV)	7.809E-09	5.069E-04	1.196E-04	1.042E-02	8.031E-02	1.226E-02	7.840E-03	0.000E+00	8.420E-06	1.872E-07	1.115E-01
Benthic Community											
Infaunal invert. (TL-II)	1.460E-10	5.733E-06	5.958E-07	1.179E-05	1.183E-05	1.083E-06	7.915E-07	0.000E+00	2.209E-09	1.574E-10	3.183E-05
Epifaunal invert. (TL-II)	2.037E-10	1.199E-05	1.431E-06	3.238E-05	3.568E-05	3.420E-06	2.525E-06	0.000E+00	6.343E-09	3.478E-10	8.744E-05
Forager (TL-III)	2.636E-10	1.456E-05	2.226E-06	6.728E-05	1.003E-04	9.375E-06	6.388E-06	0.000E+00	1.018E-08	2.336E-10	2.001E-04
Predator (TL-IV)	5.379E-11	8.946E-06	2.358E-06	1.461E-04	4.401E-04	5.295E-05	3.739E-05	0.000E+00	4.806E-08	7.065E-10	6.879E-04

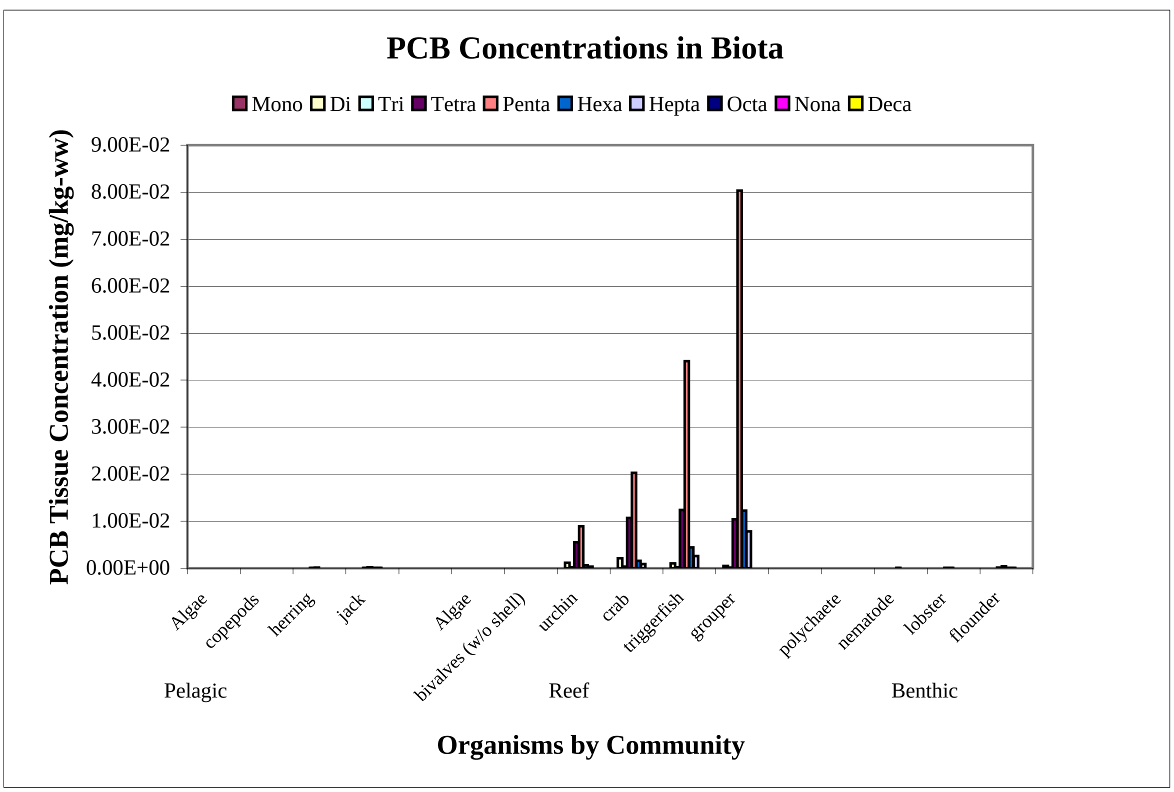
BAFs (L/kg-lipid)	Mono	Di	Tri	Tetra	Penta	Hexa	Hepta	Octa	Nona	Deca
Pelagic Community										
Phytoplankton (TL1)	2.979E+04	1.000E+05	1.000E+05	1.000E+05	1.000E+05	1.000E+05	1.000E+05	0.000E+00	1.000E+05	1.000E+05
Zooplankton (TL-II)	1.347E+05	6.238E+05	7.437E+05	8.446E+05	5.321E+05	7.827E+05	1.103E+06	0.000E+00	2.458E+06	8.127E+06
Planktivore (TL-III)	7.602E+04	1.319E+06	2.842E+06	6.256E+06	7.082E+06	1.146E+07	1.575E+07	0.000E+00	2.317E+07	2.729E+07
Piscivore (TL-IV)	1.988E+04	2.325E+05	7.546E+05	3.654E+06	1.241E+07	3.439E+07	5.326E+07	0.000E+00	6.917E+07	3.375E+07
Reef / Vessel Community										
Attached Algae	2.979E+04	1.000E+05	1.000E+05	1.000E+05	1.000E+05	1.000E+05	1.000E+05	0.000E+00	1.000E+05	1.000E+05
Sessile filter feeder (TL-II)	9.590E+05	4.034E+06	4.709E+06	5.328E+06	3.276E+06	2.983E+06	3.420E+06	0.000E+00	4.867E+06	1.181E+07
Invertebrate Omnivore (TL-II)	3.223E+04	3.116E+05	5.434E+05	1.051E+06	1.076E+06	7.781E+05	6.433E+05	0.000E+00	1.928E+05	5.351E+04
Invertebrate Forager (TL-III)	1.633E+05	8.295E+05	1.459E+06	2.957E+06	3.579E+06	2.899E+06	2.540E+06	0.000E+00	1.235E+06	1.831E+06
Vertebrate Forager (TL-III)	1.500E+04	1.310E+05	3.324E+05	1.170E+06	2.639E+06	2.736E+06	2.523E+06	0.000E+00	1.252E+06	9.322E+05
Predator (TL-IV)	1.243E+04	1.006E+05	2.806E+05	1.470E+06	7.197E+06	1.130E+07	1.144E+07	0.000E+00	5.462E+06	2.716E+06
Benthic Community										
Infaunal invert. (TL-II)	2.429E+05	1.190E+06	1.462E+06	1.740E+06	1.109E+06	1.044E+06	1.208E+06	0.000E+00	1.499E+06	2.389E+06
Epifaunal invert. (TL-II)	3.013E+05	2.213E+06	3.119E+06	4.248E+06	2.973E+06	2.930E+06	3.425E+06	0.000E+00	3.825E+06	4.691E+06
Forager (TL-III)	1.759E+05	1.212E+06	2.189E+06	3.981E+06	3.768E+06	3.622E+06	3.909E+06	0.000E+00	2.770E+06	1.421E+06
Predator (TL-IV)	1.557E+04	3.231E+05	1.006E+06	3.751E+06	7.177E+06	8.878E+06	9.928E+06	0.000E+00	5.673E+06	1.865E+06

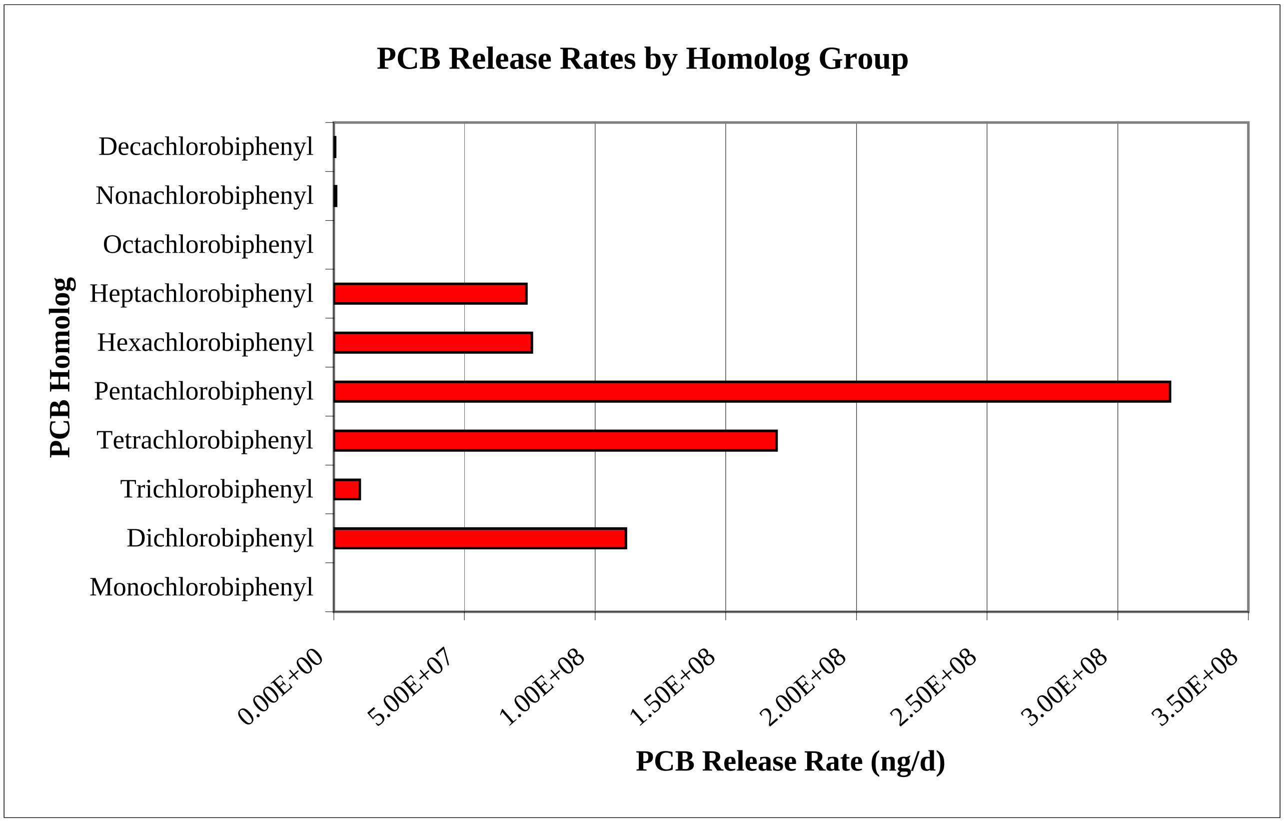
Notes:

Kow = octanol to water partitioning coefficient, Koc = organic carbon partitioning coefficient, Kdoc = dissolved organic carbon partitioning coefficient

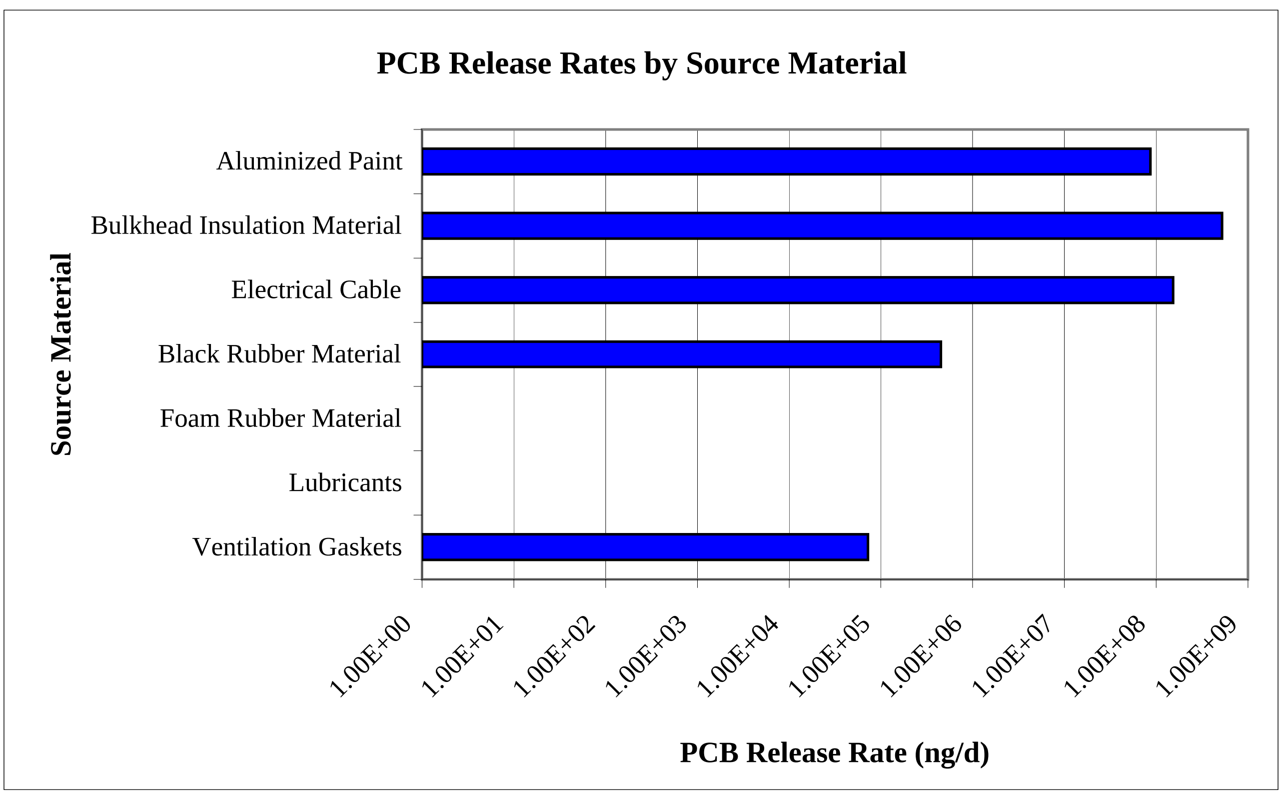
TL = trophic level, ww = wet weight


PCB Concentrations Outside the Vessel
Air concentration (g/m3)
Water Concentration-LWC (mg/L)
Suspended solids concentration-LWC (mg/kg)
Dissolved organic carbon-LWC (mg/kg)
Sediment concentration (mg/kg)
Water Concentration-UWC (mg/L)
PCB Concentration
4.00E-04
3.50E-04
3.00E-04
2.50E-04
2.00E-04
1.50E-04
1.00E-04
5.00E-05
0.00E+00
Mono
Di
Tri
Tetra
Penta
Hexa
Hepta
Octa
Nona
Deca
PCB Homolog


PCB Concentrations in Biota
Mono
Di
Tri
Tetra
Penta
Hexa
Hepta
Octa
Nona
Deca
PCB Tissue Concentration (mg/kg-ww)
9.00E-02
8.00E-02
7.00E-02
6.00E-02
5.00E-02
4.00E-02
3.00E-02
2.00E-02
1.00E-02
0.00E+00
Algae
copepods
herring
jack
Algae
bivalves (w/o shell)
urchin
crab
triggerfish
grouper
polychaete
nematode
lobster
flounder
Pelagic
Reef
Benthic
Organisms by Community



PCB Release Rates by Homolog Group
PCB Homolog
Decachlorobiphenyl
Nonachlorobiphenyl
Octachlorobiphenyl
Heptachlorobiphenyl
Hexachlorobiphenyl
Pentachlorobiphenyl
Tetrachlorobiphenyl
Trichlorobiphenyl
Dichlorobiphenyl
Monochlorobiphenyl
0.00E+00
5.00E+07
1.00E+08
1.50E+08
2.00E+08
2.50E+08
3.00E+08
3.50E+08
PCB Release Rate (ng/d)



PCB Release Rates by Source Material
Source Material
Aluminized Paint
Bulkhead Insulation Material
Electrical Cable
Black Rubber Material
Foam Rubber Material
Lubricants
Ventilation Gaskets
1.00E+00
1.00E+01
1.00E+02
1.00E+03
1.00E+04
1.00E+05
1.00E+06
1.00E+07
1.00E+08
1.00E+09
PCB Release Rate (ng/d)